

10558931.trn

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Welcome to STN International! Enter x:x

LOGINID:SSSPTA1626GMS

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * Welcome to STN International * * * * * * * * *

NEWS 1 Web Page for STN Seminar Schedule - N. America
NEWS 2 MAY 01 New CAS web site launched
NEWS 3 MAY 08 CA/CAplus Indian patent publication number format defined
NEWS 4 MAY 14 RDISCLOSURE on STN Easy enhanced with new search and display fields
NEWS 5 MAY 21 BIOSIS reloaded and enhanced with archival data
NEWS 6 MAY 21 TOXCENTER enhanced with BIOSIS reload
NEWS 7 MAY 21 CA/CAplus enhanced with additional kind codes for German patents
NEWS 8 MAY 22 CA/CAplus enhanced with IPC reclassification in Japanese patents
NEWS 9 JUN 27 CA/CAplus enhanced with pre-1967 CAS Registry Numbers
NEWS 10 JUN 29 STN Viewer now available
NEWS 11 JUN 29 STN Express, Version 8.2, now available
NEWS 12 JUL 02 LEMBASE coverage updated
NEWS 13 JUL 02 LMEDLINE coverage updated
NEWS 14 JUL 02 SCISEARCH enhanced with complete author names
NEWS 15 JUL 02 CHEMCATS accession numbers revised
NEWS 16 JUL 02 CA/CAplus enhanced with utility model patents from China
NEWS 17 JUL 16 CAplus enhanced with French and German abstracts
NEWS 18 JUL 18 CA/CAplus patent coverage enhanced
NEWS 19 JUL 26 USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 20 JUL 30 USGENE now available on STN
NEWS 21 AUG 06 CAS REGISTRY enhanced with new experimental property tags
NEWS 22 AUG 06 BEILSTEIN updated with new compounds
NEWS 23 AUG 06 FSTA enhanced with new thesaurus edition

NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * * STN. Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:18:22 ON 10 AUG 2007

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n):

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST | 0.21 | 0.21 |

FILE 'REGISTRY' ENTERED AT 14:18:31 ON 10 AUG 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 9 AUG 2007 HIGHEST RN 944380-35-2

DICTIONARY FILE UPDATES: 9 AUG 2007 HIGHEST RN 944380-35-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

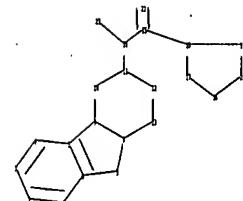
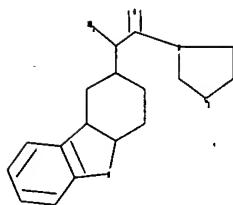
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

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chain nodes :

14 15 22 23

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 16 17 18 19 20

chain bonds :

11-14 14-15 14-23 15-18 15-22

ring bonds :

1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13
16-17 16-20 17-18 18-19 19-20

exact/norm bonds :

5-8 5-6 7-9 8-13 8-9 9-10 10-11 11-12 11-14 12-13 14-15 14-23 15-18
15-22 16-17 16-20 17-18 18-19 19-20

normalized bonds :

1-2 1-6 2-3 3-4 4-7 6-7

isolated ring systems :

containing 1 : 16 :

G1:S,CH2,CH,CF2,SO2

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 22:CLASS 23:CLASS

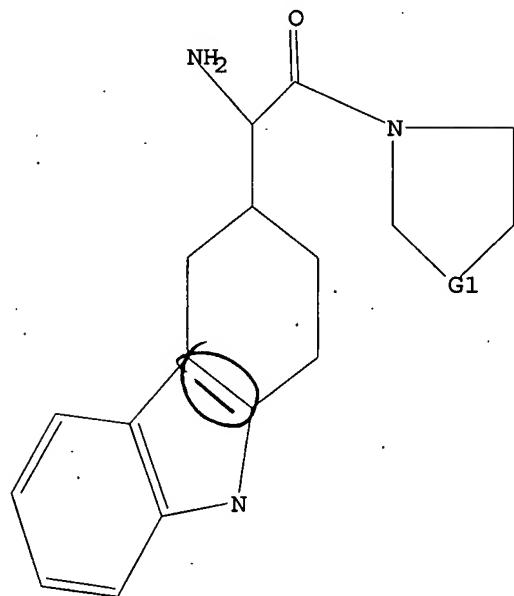
10558931.trn

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 14:18:46 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 0 TO 0

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 14:18:53 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 52 TO ITERATE

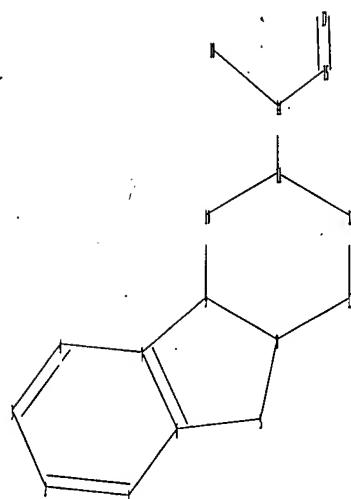
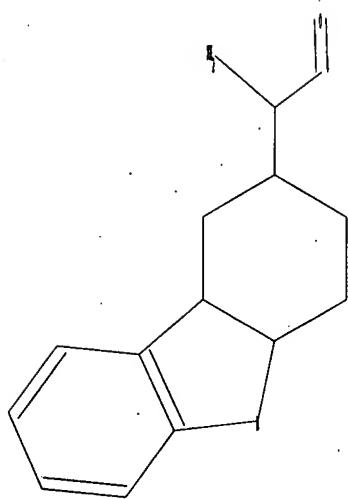
100.0% PROCESSED 52 ITERATIONS
SEARCH TIME: 00.00.01

0 ANSWERS

L3 0 SEA SSS FUL L1

=>

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chain nodes :

14 15 17 18

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

chain bonds :

11-14 14-15 14-18 15-17

ring bonds :

1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10, 10-11 11-12 12-13

exact/norm bonds :

5-8 5-6 14-18 15-17

exact bonds :

7-9 8-13 8-9 9-10 10-11 11-12 11-14 12-13 14-15

normalized bonds :

1-2 1-6 2-3 3-4 4-7 6-7

isolated ring systems :

containing 1 :

G1:S,CH2,CH,CF2,SO2

Match level :

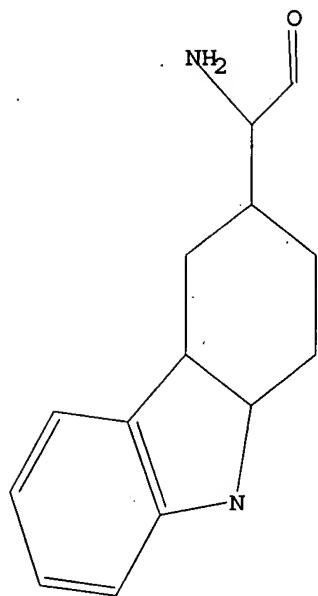
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 17:CLASS 18:CLASS

L4 STRUCTURE UPLOADED

=> d.14

L4 HAS NO ANSWERS

L4 STR



G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

=> s 14
SAMPLE SEARCH INITIATED 14:20:09 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 39 TO ITERATE

100.0% PROCESSED 39 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 406 TO 1154
PROJECTED ANSWERS: 0 TO 0

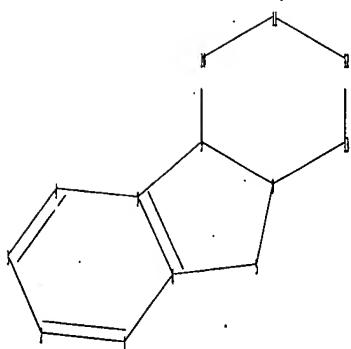
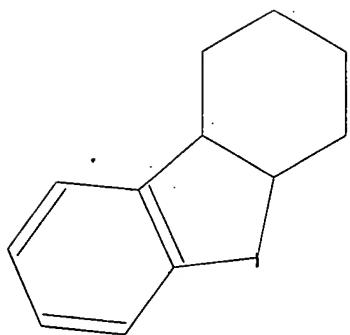
L5 0 SEA SSS SAM L4

=> s 14 sss full
FULL SEARCH INITIATED 14:20:15 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 740 TO ITERATE

100.0% PROCESSED 740 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L6 0 SEA SSS FUL L4

=>
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ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

ring bonds :

1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13

exact/norm bonds :

5-8 5-6

exact bonds :

7-9 8-13 8-9 9-10 10-11 11-12 12-13

normalized bonds :

1-2 1-6 2-3 3-4 4-7 6-7

isolated ring systems :

containing 1 :

G1:S,CH2,CH,CF2,SO2

Match level :

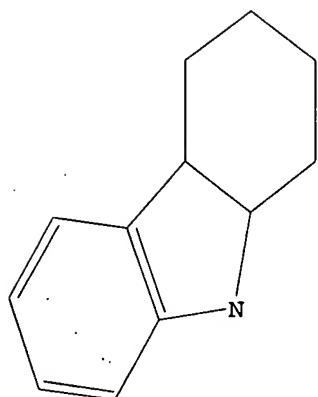
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom

L7 STRUCTURE UPLOADED

=> d 17

L7 HAS NO ANSWERS

L7 STR



G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

=> s 17
SAMPLE SEARCH INITIATED 14:21:33 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 2011 TO ITERATE

99.5% PROCESSED 2000 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 37530 TO 42910
PROJECTED ANSWERS: 740 TO 1672

L8 50 SEA SSS SAM L7

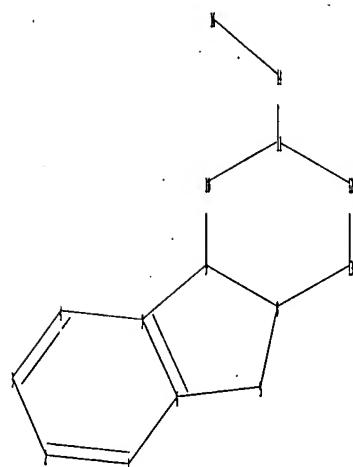
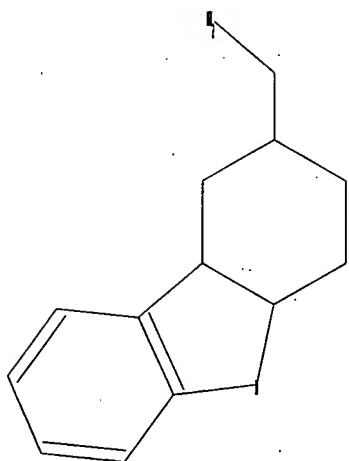
=> s 17 sss full
FULL SEARCH INITIATED 14:21:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 38933 TO ITERATE

100.0% PROCESSED 38933 ITERATIONS 1220 ANSWERS
SEARCH TIME: 00.00.01

L9 1220 SEA SSS FUL L7

=>
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10558931.trn



chain nodes :

14 16

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

chain bonds :

11-14 14-16

ring bonds :

1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13

exact/norm bonds :

5-8 5-6 14-16

exact bonds :

7-9 8-13 8-9 9-10 10-11 11-12 11-14 12-13

normalized bonds :

1-2 1-6 2-3 3-4 4-7 6-7

isolated ring systems :

containing 1 :

G1:S,CH2,CH,CF2,SO2

Match level :

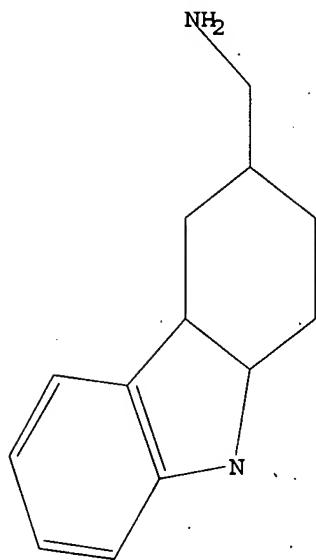
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 16:CLASS

L10 STRUCTURE UPLOADED

=> d l10

L10 HAS NO ANSWERS

L10 STR



G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

=> s 110
SAMPLE SEARCH INITIATED 14:22:55 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 216 TO ITERATE
100.0% PROCESSED 216 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 3439 TO 5201
PROJECTED ANSWERS: 0 TO 0

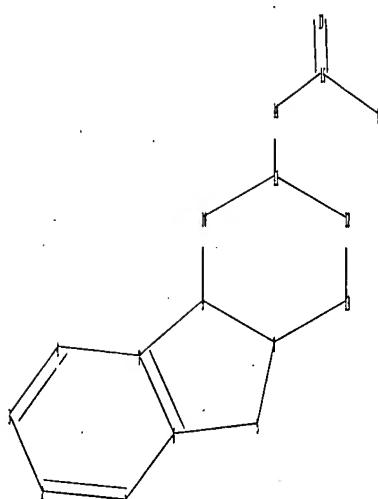
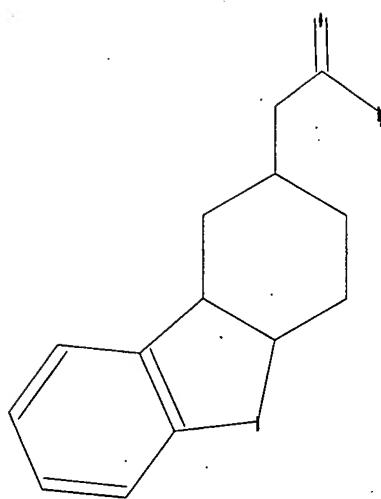
L11 0 SEA SSS SAM L10

=> s 110 sss full
FULL SEARCH INITIATED 14:23:01 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3888 TO ITERATE

100.0% PROCESSED 3888 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

L12 0 SEA SSS FUL L10

=>
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chain nodes :

14 15 17 19

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

chain bonds :

11-14 14-15 15-17 15-19

ring bonds :

1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13

exact/norm bonds :

5-8 5-6 15-17 15-19

exact bonds :

7-9 8-13 8-9 9-10 10-11 11-12 11-14 12-13 14-15

normalized bonds :

1-2 1-6 2-3 3-4 4-7 6-7

isolated ring systems :

containing 1 :

G1:S,CH2,CH,CF2,SO2

Match level :

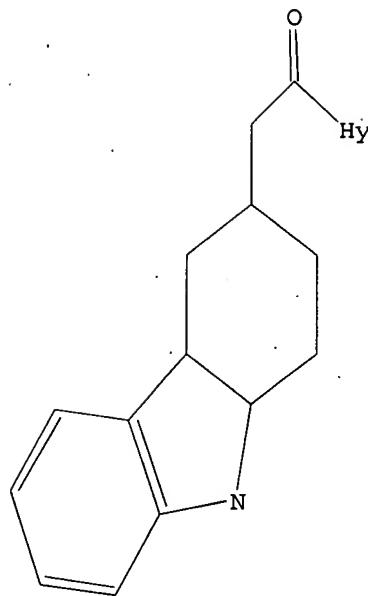
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 17:CLASS 19:CLASS

L13 STRUCTURE UPLOADED

=> d 113

L13 HAS NO ANSWERS

L13 STR



G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

```
=> s 113
SAMPLE SEARCH INITIATED 14:24:43 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 244 TO ITERATE

100.0% PROCESSED      244 ITERATIONS          0 ANSWERS
SEARCH TIME: .00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH **COMPLETE**
PROJECTED ITERATIONS:    3943 TO      5817
PROJECTED ANSWERS:        0 TO       0

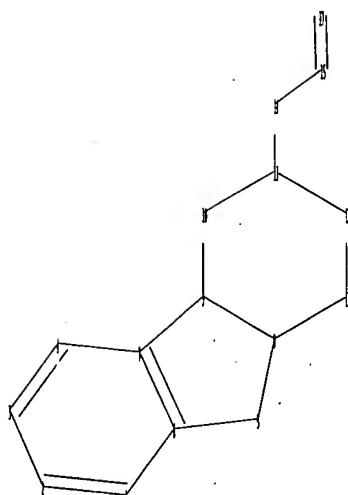
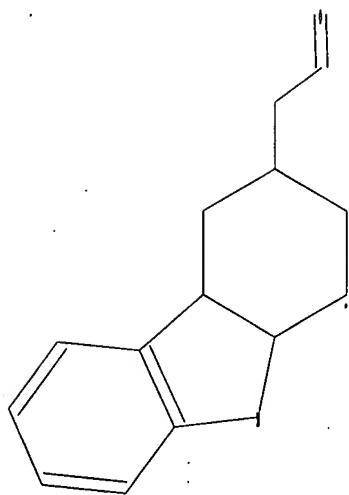
L14      0 SEA SSS SAM L13

=> s 113 sss full
FULL SEARCH INITIATED 14:24:50 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4979 TO ITERATE

100.0% PROCESSED      4979 ITERATIONS          0 ANSWERS
SEARCH TIME: .00.00.01

L15      0 SEA SSS FUL L13

=>
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```



chain nodes :

14 15 17

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

chain bonds :

11-14 14-15 15-17

ring bonds :

1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13

exact/norm bonds :

5-8 5-6 15-17

exact bonds :

7-9 8-13 8-9 9-10 10-11 11-12 11-14 12-13 14-15

normalized bonds :

1-2 1-6 2-3 3-4 4-7 6-7

isolated ring systems :

containing 1 :

G1:S,CH2,CH,CF2,SO2

Match level :

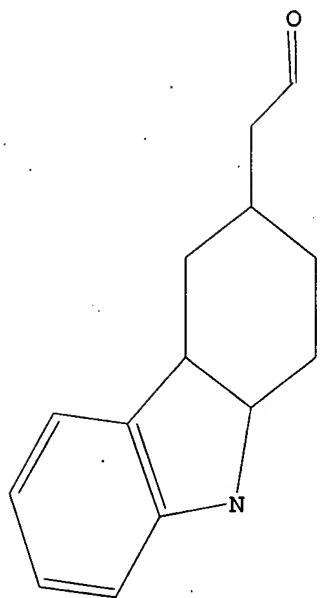
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 17:CLASS

L16 STRUCTURE UPLOADED

=> d 116

L16 HAS NO ANSWERS

L16 STR



G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

```
=> s 116
SAMPLE SEARCH INITIATED 14:27:21 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 244 TO ITERATE

100.0% PROCESSED 244 ITERATIONS
SEARCH TIME: 00.00.01
```

0 ANSWERS

```
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 3943 TO 5817
PROJECTED ANSWERS: 0 TO 0
```

L17 0 SEA SSS SAM L16

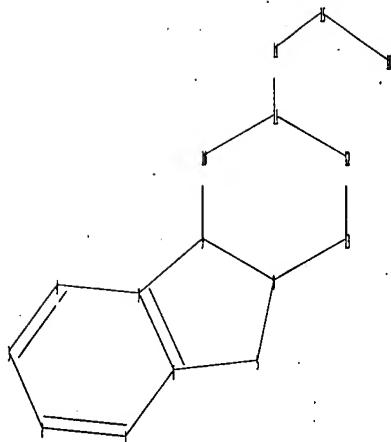
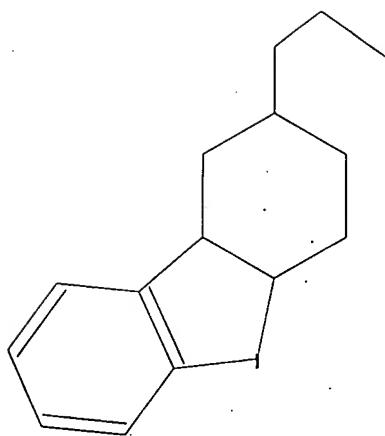
```
=> s 116 sss full
FULL SEARCH INITIATED 14:27:29 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 4979 TO ITERATE
```

```
100.0% PROCESSED 4979 ITERATIONS
SEARCH TIME: 00.00.01
```

0 ANSWERS

L18 0 SEA SSS FUL L16

```
=>
Uploading C:\Program Files\Stnexp\Queries\10558931f.str
```



chain nodes :

14 15 18

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

chain bonds :

11-14 14-15 15-18

ring bonds :

1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13

exact/norm bonds :

5-8 5-6 15-18

exact bonds :

7-9 8-13 8-9 9-10 10-11 11-12 11-14 12-13 14-15

normalized bonds :

1-2 1-6 2-3 3-4 4-7 6-7

isolated ring systems :

containing 1 :

G1:S,CH2,CH,CF2,SO2

Match level :

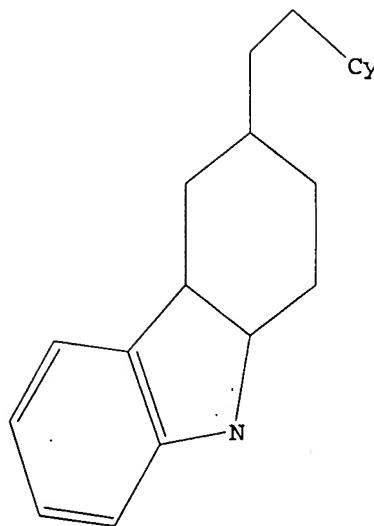
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 18:CLASS

L19 STRUCTURE UPLOADED

=> d 119

L19 HAS NO ANSWERS

L19 STR



G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

=> s 119

SAMPLE SEARCH INITIATED 14:30:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 954 TO ITERATE

100.0% PROCESSED 954 ITERATIONS
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 17227 TO 20933

PROJECTED ANSWERS: 0 TO 0

L20 0 SEA SSS SAM L19

=> s 119 sss full

FULL SEARCH INITIATED 14:30:11 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 17864 TO ITERATE

100.0% PROCESSED 17864 ITERATIONS
SEARCH TIME: 00.00.01

0 ANSWERS

L21 0 SEA SSS FUL L19

=> d his

(FILE 'HOME' ENTERED AT 14:18:22 ON 10 AUG 2007)

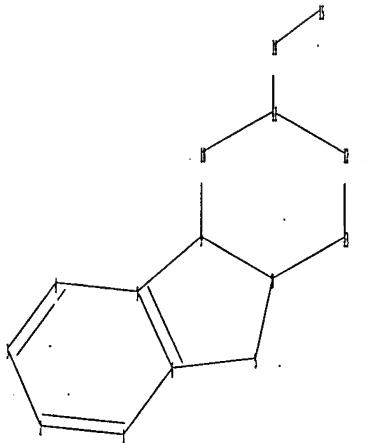
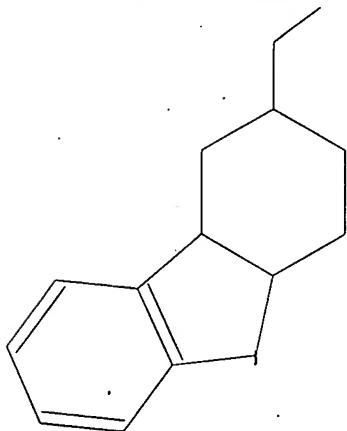
FILE 'REGISTRY' ENTERED AT 14:18:31 ON 10 AUG 2007

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 0 S L1 SSS FULL
L4 STRUCTURE UPLOADED
L5 0 S L4

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L6 0 S L4 SSS FULL
L7 STRUCTURE UPLOADED
L8 50 S L7
L9 1220 S L7 SSS FULL
L10 STRUCTURE UPLOADED
L11 0 S L10
L12 0 S L10 SSS FULL
L13 STRUCTURE UPLOADED
L14 0 S L13
L15 0 S L13 SSS FULL
L16 STRUCTURE UPLOADED
L17 0 S L16
L18 0 S L16 SSS FULL
L19 STRUCTURE UPLOADED
L20 0 S L19
L21 0 S L19 SSS FULL

=>
Uploading C:\Program Files\Stnexp\Queries\10558931g.str



chain nodes :

14 15

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13

chain bonds :

11-14 14-15

ring bonds :

1-2 1-6 2-3 3-4 4-7 5-8 5-6 6-7 7-9 8-13 8-9 9-10 10-11 11-12 12-13

exact/norm bonds :

5-8 5-6

exact bonds :

7-9 8-13 8-9 9-10 10-11 11-12 11-14 12-13 14-15

normalized bonds :

1-2 1-6 2-3 3-4 4-7 6-7

isolated ring systems :

containing 1 :

G1:S,CH2,CH,CF2,SO2

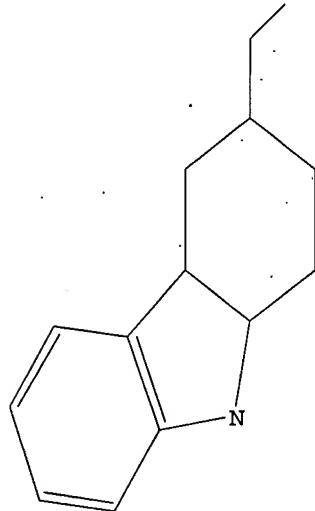
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS

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L22 STRUCTURE UPLOADED

=> d 122
L22 HAS NO ANSWERS
L22 STR



G1 S,CH2,CH,CF2,SO2

Structure attributes must be viewed using STN Express query preparation.

=> s 122
SAMPLE SEARCH INITIATED 14:32:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1082 TO ITERATE

100.0% PROCESSED 1082 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 19667 TO 23613
PROJECTED ANSWERS: 2 TO 124

L23 2 SEA SSS SAM L22

=> s 122 sss full
FULL SEARCH INITIATED 14:32:30 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 20417 TO ITERATE

100.0% PROCESSED 20417 ITERATIONS 36 ANSWERS
SEARCH TIME: 00.00.01

L24 36 SEA SSS FUL L22

=> d his

10558931.trn

(FILE 'HOME' ENTERED AT 14:18:22 ON 10 AUG 2007)

FILE 'REGISTRY' ENTERED AT 14:18:31 ON 10 AUG 2007

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 0 S L1 SSS FULL
L4 STRUCTURE UPLOADED
L5 0 S L4
L6 0 S L4 SSS FULL
L7 STRUCTURE UPLOADED
L8 50 S L7
L9 1220 S L7 SSS FULL
L10 STRUCTURE UPLOADED
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L16 STRUCTURE UPLOADED
L17 0 S L16
L18 0 S L16 SSS FULL
L19 STRUCTURE UPLOADED
L20 0 S L19
L21 0 S L19 SSS FULL
L22 STRUCTURE UPLOADED
L23 2 S L22
L24 36 S L22 SSS FULL

=> FIL HCAPLUS

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST | 1384.00 | 1384.21 |

FILE 'HCAPLUS' ENTERED AT 14:33:02 ON 10 AUG 2007
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FILE COVERS 1907 - 10 Aug 2007 VOL 147 ISS 8
FILE LAST UPDATED: 9 Aug 2007 (20070809/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 124
L25 15 L24

10558931.trn

=> s 19
L26 472 L9

=> s 125 and py<=2003
23927587 PY<=2003
L27 14 L25 AND PY<=2003

=> s 126 and p/dt
5818845 P/DT
L28 127 L26 AND P/DT

=> s 128 and us/pc
1705037 US/PC
L29 57 L28 AND US/PC

=> s 129 and py<=2003
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=> s 130 and dipeptidyl
4690 DIPEPTIDYL
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=> s 130 and thu
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2428717 THUS
2428858 THU
(THU OR THUS)
L32 28 L30 AND THU

=> s 132 and diabetes
128376 DIABETES
L33 0 L32 AND DIABETES

=> s 132 and disease
978988 DISEASE
264275 DISEASES
1096696 DISEASE
(DISEASE OR DISEASES)
L34 4 L32 AND DISEASE

=> d his

(FILE 'HOME' ENTERED AT 14:18:22 ON 10 AUG 2007)

FILE 'REGISTRY' ENTERED AT 14:18:31 ON 10 AUG 2007

L1 STRUCTURE UPLOADED
L2 0 S L1
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10558931.trn

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FILE 'HCAPLUS' ENTERED AT 14:33:02 ON 10 AUG 2007

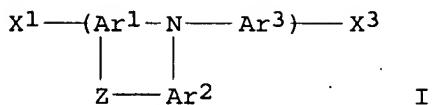
L25 15 S L24
L26 472 S L9
L27 14 S L25 AND PY<=2003
L28 127 S L26 AND P/DT
L29 57 S L28 AND US/PC
L30 51 S L29 AND PY<=2003
L31 0 S L30 AND DIPEPTIDYL
L32 28 S L30 AND THU
L33 0 S L32 AND DIABETES
L34 4 S L32 AND DISEASE

=> d l25 ibib abs hitstr tot

L25 ANSWER 1 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:656254 HCAPLUS
DOCUMENT NUMBER: 145:125169
TITLE: Rigid amines for use in manufacture of conjugated polymer useful as emitters, charge transporters or host materials in opto-electrical devices
INVENTOR(S): Heidenhain, Sophie; Leadbeater, Mark; Steudel, Annette; Hicks, Daniel
PATENT ASSIGNEE(S): Cambridge Display Technology Limited, UK; CDT Oxford Limited
SOURCE: PCT Int. Appl., 49 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| WO 2006070185 | A1 | 20060706 | WO 2005-GB5058 | 20051223 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,
KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
VN, YU, ZA, ZM, ZW | | | | |
| RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM | | | | |
| PRIORITY APPLN. INFO.: | | | GB 2004-28443 | A 20041229 |
| | | | GB 2005-2254 | A 20050203 |

GI

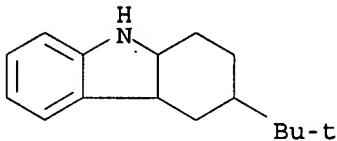


AB The monomer has a structure as shown in I where: Ar1, Ar2 and Ar3 are independently selected from optionally substituted aryl or heteroaryl, X1 and X3 both independently comprise a leaving group capable of participating in polymerization and Z represents a direct bond or an optionally substituted bridging atom.

IT 6731-89-1P
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
 (manufacture of rigid amines as monomers for conjugated polymer useful for emitters, charge transporters or host materials in opto-elec. devices)

RN 6731-89-1 HCPLUS

CN 1H-Carbazole, 3-(1,1-dimethylethyl)-2,3,4,4a,9,9a-hexahydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 2 OF 15 HCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1999:363554 HCPLUS
 DOCUMENT NUMBER: 131:115858
 TITLE: Alkylation of ketone and ester lithium enolates with nitroethylene
 AUTHOR(S): Flintoft, Rebecca J.; Buzby, Jennifer C.; Tucker, John A.
 CORPORATE SOURCE: Medicinal Chemistry Research, Pharmacia and Upjohn, Kalamazoo, MI, 49001, USA
 SOURCE: Tetrahedron Letters (1999), 40(24), 4485-4488
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 131:115858

AB We describe the first systematic study of the scope and limitations of the conjugate addition of ketone and ester enolates to nitroethylene. Synthetically useful yields are obtained for ketone and ester enolates of a variety of structural types.

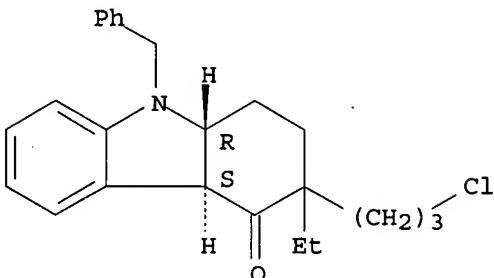
IT 232923-95-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (alkylation of ketone enolates or ester enolates with nitroethylene)

RN 232923-95-4 HCPLUS

CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-9-

(phenylmethyl)-, (4aR,9aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 232924-06-0P

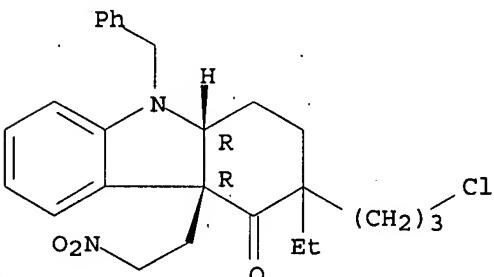
RL: SPN (Synthetic preparation); PREP (Preparation)

(alkylation of ketone enolates or ester enolates with nitroethylene)

RN 232924-06-0 HCPLUS

CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-(2-nitroethyl)-9-(phenylmethyl)-, (4aR,9aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT:

22

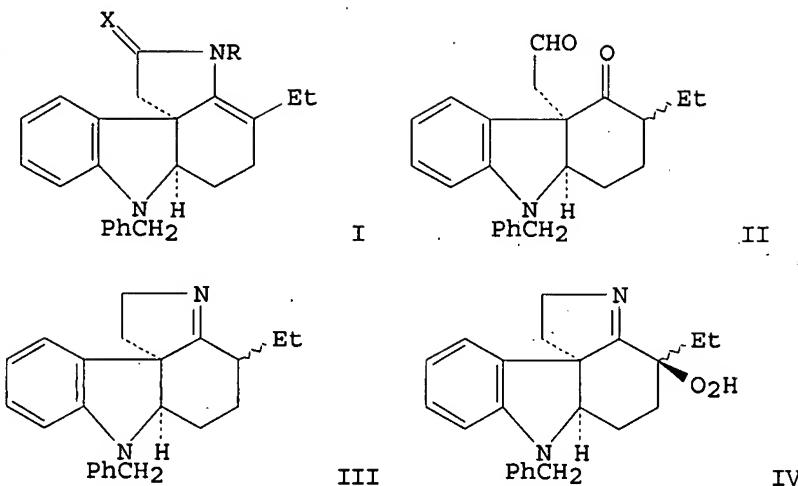
THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 3 OF 15 HCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:631122 HCPLUS

DOCUMENT NUMBER: 121:231122

TITLE: Unexpected results in the reduction of tetracyclic enamides. Structure, stereochemistry and conformation of a 20 β -hydroperoxyimineAUTHOR(S): Dugat, Denise; Dauphin, Gerard; Gramain, Jean-Claude
CORPORATE SOURCE: Universite Blaise Pascal de Clermont-Ferrand, Aubiere, 63177, Fr.SOURCE: Heterocycles (1994), 38(8), 1909-18
CODEN: HTCYAM; ISSN: 0385-5414DOCUMENT TYPE: Journal
LANGUAGE: English
GI



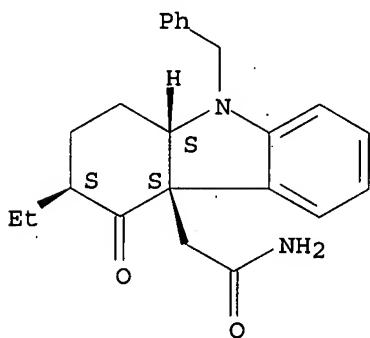
AB Reduction of Nb-allyl-20-ethyltetracyclic enamide I ($X = O$, $R = \text{allyl}$) with lithium aluminum hydride afforded the expected enamine I ($X = H_2$, $R = \text{allyl}$) and 4a-oxoethylhexahydrocarbazolones II. Reduction of Nb-unsubstituted enamide I ($X = O$, $R = H$), under the same conditions, gave imine III, enamine I ($X = H_2$, $R = H$) and a 20 β -hydroperoxytetracyclic imine IV resulting from peroxydation. The C-20 stereochem. of IV was established by means of 2D 1H NMR and NOE difference spectroscopy.

IT 158148-36-8P 158148-37-9P 158148-38-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and intramol. cyclization of)

RN 158148-36-8 HCPLUS

CN 4aH-Carbazole-4a-acetamide, 3-ethyl-1,2,3,4,9,9a-hexahydro-4-oxo-9-(phenylmethyl)-, (3 α ,4 $\alpha\alpha$,9 $\alpha\alpha$)- (9CI) (CA INDEX NAME)

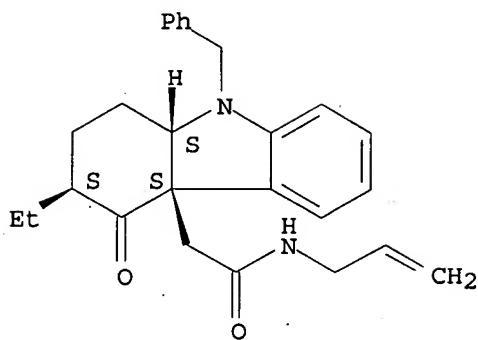
Relative stereochemistry.



RN 158148-37-9 HCPLUS

CN 4aH-Carbazole-4a-acetamide, 3-ethyl-1,2,3,4,9,9a-hexahydro-4-oxo-9-(phenylmethyl)-N-2-propenyl-, (3 α ,4 $\alpha\alpha$,9 $\alpha\alpha$)- (9CI) (CA INDEX NAME)

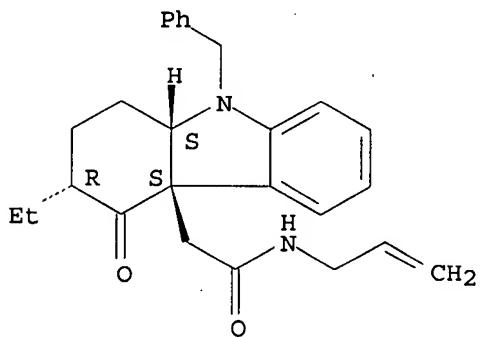
Relative stereochemistry.



RN 158148-38-0 HCPLUS

CN 4aH-Carbazole-4a-acetamide, 3-ethyl-1,2,3,4,9,9a-hexahydro-4-oxo-9-(phenylmethyl)-N-2-propenyl-, (3 α ,4a β ,9a β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



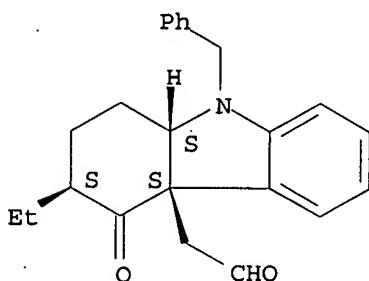
IT 158148-44-8P 158148-45-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 158148-44-8 HCPLUS

CN 4aH-Carbazole-4a-acetaldehyde, 3-ethyl-1,2,3,4,9,9a-hexahydro-4-oxo-9-(phenylmethyl)-, (3 α ,4a α ,9a α)- (9CI) (CA INDEX NAME)

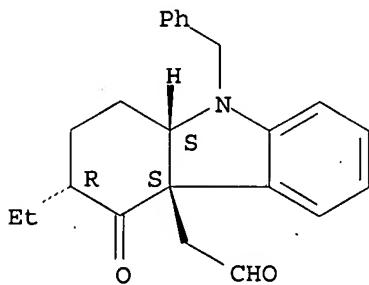
Relative stereochemistry.



RN 158148-45-9 HCPLUS

CN 4aH-Carbazole-4a-acetaldehyde, 3-ethyl-1,2,3,4,9,9a-hexahydro-4-oxo-9-(phenylmethyl)-, (3 α ,4a β ,9a β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



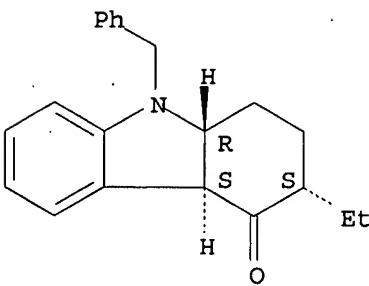
IT 129574-42-1

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with iodoacetamide)

RN 129574-42-1 HCPLUS

CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-,
(3 α ,4 α ,9 α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



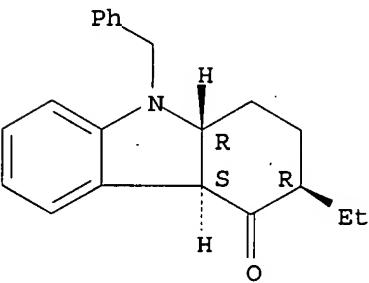
IT 129574-41-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with iodoacetamides)

RN 129574-41-0 HCPLUS

CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-,
(3 α ,4 β ,9 α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



10558931.trn

DOCUMENT NUMBER: 120:134890
TITLE: Stereocontrolled formation of octahydro-1H-pyrrolo[2,3-d]carbazoles by reductive cyclization: total synthesis of (\pm)-N-benzylaspidospermidine
AUTHOR(S): Benchekroun-Mounir, Nora; Dugat, Denise; Gramain, Jean Claude; Husson, Henri Philippe
CORPORATE SOURCE: URA, Univ. Blaise Pascal Clermont-Ferrand, Aubiere, 63177, Fr.
SOURCE: Journal of Organic Chemistry (1993), 58(23), 6457-65
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:134890
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The synthesis of a series of 20-substituted octahydro-1H-pyrrolo[2,3-d]carbazoles, intermediates in the synthesis of Aspidosperma alkaloids, is described. Nonoxidative photocyclization of aryl enaminone I led to hexahydrocarbazol-4-ones II. Alkylation of the anions derived from II with KH and iodoacetonitrile gave rise to an undesirable intramol. cyclization while reaction with LDA and nitroethylene as Michael acceptor afforded the trisubstituted hexahydrocarbazolones III (R = CH₂CH₂CH₂Cl). Reductive cyclization (H₂, PtO₂) of cyano model compds. provided octahydro-1H-pyrrolo[2,3-d]carbazoles whose stereochem. depended on hindrance of the α and β face of the mol. In contrast, reduction (HCOONH₄, Pd/C, and then Na/EtOH) of nitro model compds. III (R = H) via nitrones led essentially to the more stable isomers IV with the natural stereochem. at C-21. Reduction (HCOONH₄, Pd/C) of nitro compds. III (R = CH₂CH₂CH₂Cl), which possess the elements for the future construction of the D and E rings, induced a tandem cyclization and afforded the pentacyclic iminium which was converted by catalytic hydrogenation into (\pm)-N-benzylaspidospermidine (V). This compound was thus synthesized in seven steps from N-benzyylaniline and cyclohexane-1,3-dione.

IT 129574-41-0 129574-43-2

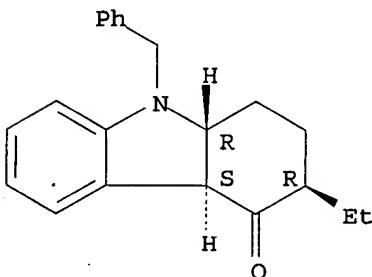
RL: PROC (Process)

(addition of, with nitroethylene)

RN 129574-41-0 HCPLUS

CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3 α ,4a β ,9 α)- (9CI) (CA INDEX NAME)

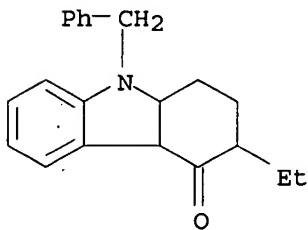
Relative stereochemistry.



RN 129574-43-2 HCPLUS

10558931.trn

CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3 α ,4 $\alpha\alpha$,9 $\alpha\alpha$)- (9CI) (CA INDEX NAME)



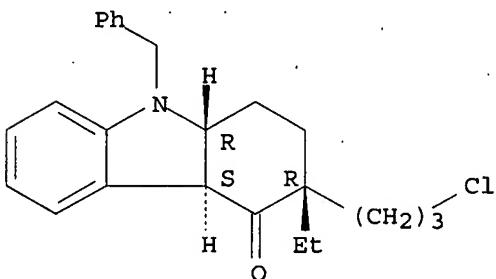
IT 143466-44-8P 143466-49-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and addition of, with nitroethylene)

RN 143466-44-8 HCAPLUS

CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3 α ,4 $\alpha\beta$,9 $\alpha\beta$)- (9CI) (CA INDEX NAME)

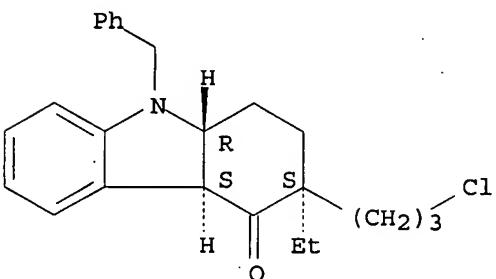
Relative stereochemistry.



RN 143466-49-3 HCAPLUS

CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3 α ,4 $\alpha\beta$,9 $\alpha\alpha$)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 152710-80-0P 152710-81-1P 152710-89-9P

152710-90-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(preparation and reduction of)

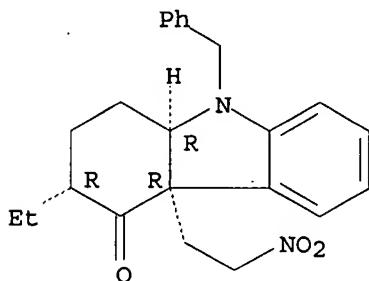
RN 152710-80-0 HCAPLUS

CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-(2-nitroethyl)-9-

10558931.trn

(phenylmethyl)-, (3 α ,4 $\alpha\alpha$,9 $\alpha\alpha$)- (9CI) (CA INDEX NAME)

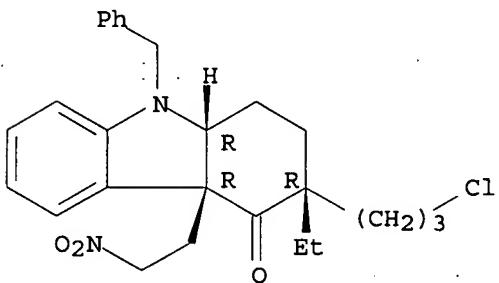
Relative stereochemistry.



RN 152710-81-1 HCPLUS

CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-(2-nitroethyl)-9-(phenylmethyl)-, (3 α ,4 $\alpha\beta$,9 $\alpha\beta$)- (9CI) (CA INDEX NAME)

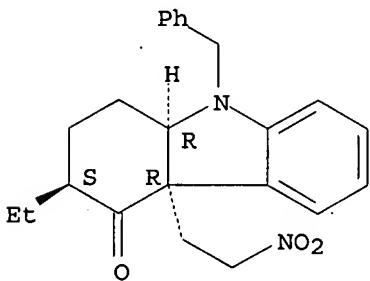
Relative stereochemistry.



RN 152710-89-9 HCPLUS

CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-(2-nitroethyl)-9-(phenylmethyl)-, (3 α ,4 $\alpha\beta$,9 $\alpha\beta$)- (9CI) (CA INDEX NAME)

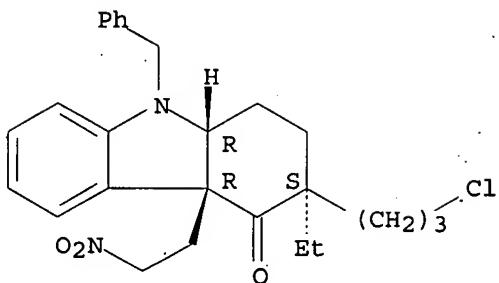
Relative stereochemistry.



RN 152710-90-2 HCPLUS

CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-(2-nitroethyl)-9-(phenylmethyl)-, (3 α ,4 $\alpha\alpha$,9 $\alpha\alpha$)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



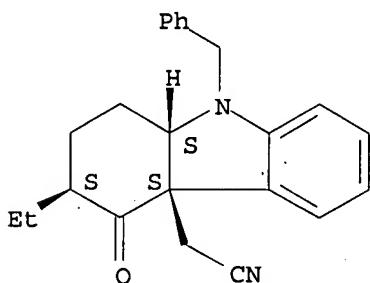
IT 152710-78-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reductive intramol. cyclization of)

RN 152710-78-6 HCAPLUS

CN 4aH-Carbazole-4a-acetonitrile, 3-ethyl-1,2,3,4,9,9a-hexahydro-4-oxo-9-(phenylmethyl)-, (3 α ,4 $\alpha\alpha$,9 $\alpha\alpha$)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



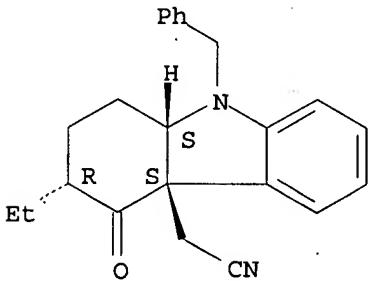
IT 152710-88-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 152710-88-8 HCAPLUS

CN 4aH-Carbazole-4a-acetonitrile, 3-ethyl-1,2,3,4,9,9a-hexahydro-4-oxo-9-(phenylmethyl)-, (3 α ,4 $\alpha\beta$,9 $\alpha\beta$)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



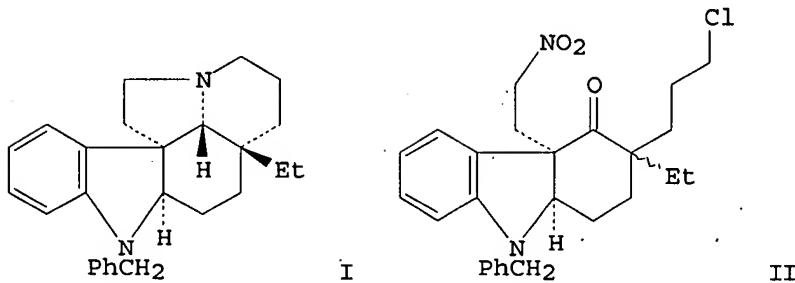
L25 ANSWER 5 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1992:571783 HCAPLUS

DOCUMENT NUMBER: 117:171783

TITLE: A short synthesis of (\pm)-N-benzyl aspidospermidine

AUTHOR(S): Benchekroun-Mounir, Nora; Dugat, Denise; Gramain, Jean Claude
 CORPORATE SOURCE: Univ. Blaise Pascal de Clermont-Ferrand, Aubiere,
 63177, Fr.
 SOURCE: Tetrahedron Letters (1992), 33(28), 4001-4
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 117:171783
 GI



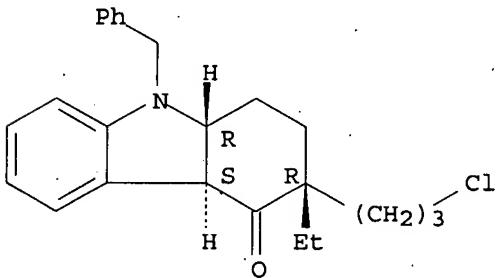
AB (±)-N-Benzyl aspidospermidine (I) is synthesized in seven steps via the trisubstituted hexahydrocarbazolone II; reductive cyclization of this intermediate which is obtained by photocyclization and Michael reaction with nitroethylene, creates simultaneously both E and D rings of the pentacyclic system.

IT 143466-44-8P 143466-49-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and alkylation of, with nitroethylene)

RN 143466-44-8 HCAPLUS

CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3 α ,4a α ,9a β)- (9CI) (CA INDEX NAME)

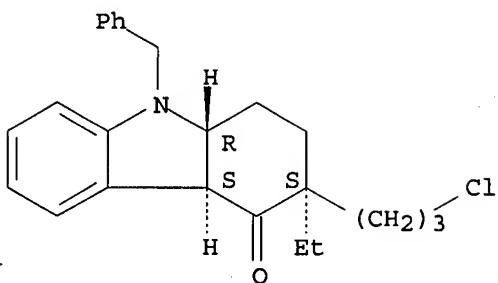
Relative stereochemistry.



RN 143466-49-3 HCAPLUS

CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3 α ,4a β ,9a α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



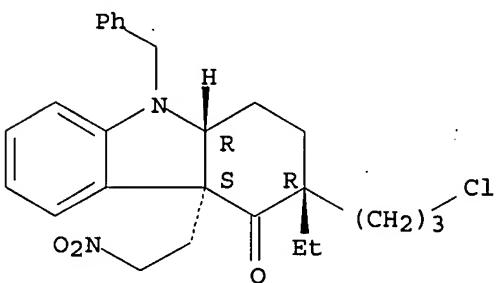
IT 143466-45-9P 143466-48-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reductive cyclization of)

RN 143466-45-9 HCPLUS

CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-(2-nitroethyl)-9-(phenylmethyl)-, (3 α ,4 $\alpha\alpha$,9 $\alpha\beta$)- (9CI)
(CA INDEX NAME)

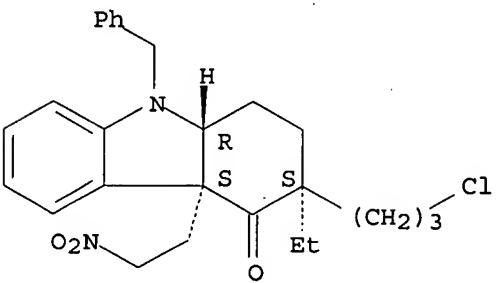
Relative stereochemistry.



RN 143466-48-2 HCPLUS

CN 4H-Carbazol-4-one, 3-(3-chloropropyl)-3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-(2-nitroethyl)-9-(phenylmethyl)-, (3 α ,4 $\alpha\beta$,9 $\alpha\alpha$)- (9CI)
(CA INDEX NAME)

Relative stereochemistry.



L25 ANSWER 6 OF 15 HCPLUS COPYRIGHT 2007 ACS on STN

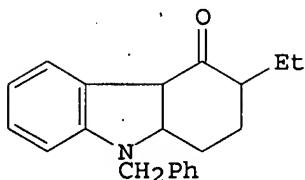
ACCESSION NUMBER: 1990:552186 HCPLUS

DOCUMENT NUMBER: 113:152186

TITLE: Structure, stereochemistry, and conformation of

diastereoisomeric cis- and trans-3-ethyl-1,2,3,4,4a,9a-hexahydrocarbazol-4-ones by means of ^{13}C and two-dimensional proton NMR spectroscopy. An example

AUTHOR(S): Dugat, Denise; Gramain, Jean Claude; Dauphin, Gerard
 CORPORATE SOURCE: Unite Rech., Univ. Blaise Pascal Clermont-Ferrand, Aubiere, 63177, Fr.
 SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1990), (4), 605-11
 DOCUMENT TYPE: CODEN: JCPKBH; ISSN: 0300-9580
 LANGUAGE: Journal English
 OTHER SOURCE(S): CASREACT 113:152186
 GI



I

AB Diastereoisomers of 3-ethylhexahydrocarbazol-4-one (I) are stereospecifically obtained in a 4a,9a-trans-configuration by a photocyclization reaction in which appreciable diastereoselection (40%) due to the Et chain is observed. They are quant. converted to cis compds: by treatment with acid or by angular alkylation via a benzylic carbanion. Complete anal. of the ^1H (1D, 2D) NMR spectra allows the conformation of the C ring in each compound to be established. Moreover, the collected ^1H and ^{13}C NMR data constitute refs. for further identification of the cis and trans series and further determination of the position of the 3-Et chain. Equilibrium studies between the different isomers show the higher stability of the cis derivs. which possess the configuration of the natural products of the Aspidosperma indole alkaloids.

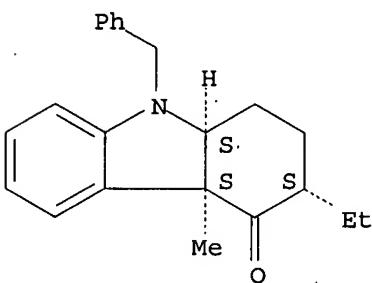
IT 129574-45-4 129574-46-5

RL: RCT (Reactant); RACT (Reactant or reagent)
 (NMR of carbon-13 and hydrogen in)

RN 129574-45-4 HCPLUS

CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-methyl-9-(phenylmethyl)-, (3 α ,4 α ,9 α)- (9CI) (CA INDEX NAME)

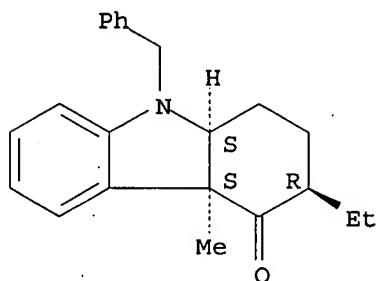
Relative stereochemistry.



10558931.trn

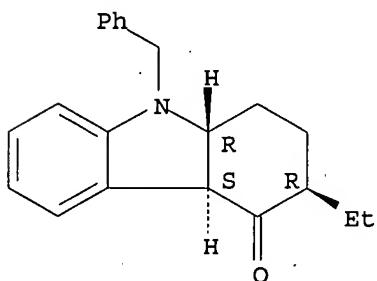
RN 129574-46-5 HCAPLUS
CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-4a-methyl-9-(phenylmethyl)-, (3 α ,4a β ,9a β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



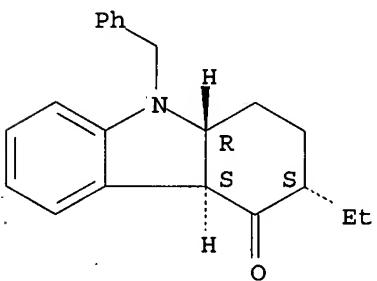
IT 129574-41-0P 129574-42-1P 129574-43-2P
129574-44-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and NMR of)
RN 129574-41-0 HCAPLUS
CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-,
(3 α ,4a β ,9a α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

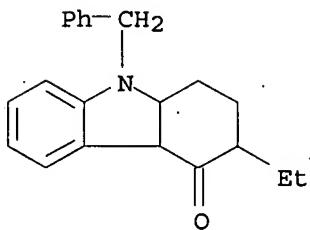


RN 129574-42-1 HCAPLUS
CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-,
(3 α ,4a α ,9a β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



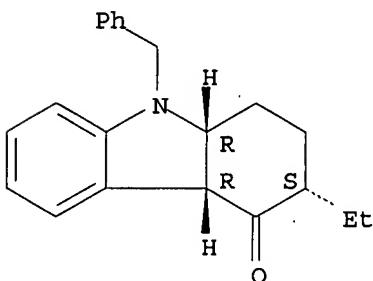
RN 129574-43-2 HCAPLUS
CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-,

(3 α ,4 α ,9 α)- (9CI) (CA INDEX NAME)

RN 129574-44-3 HCPLUS

CN 4H-Carbazol-4-one, 3-ethyl-1,2,3,4a,9,9a-hexahydro-9-(phenylmethyl)-, (3 α ,4 α β ,9 α β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L25 ANSWER 7 OF 15 HCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1987:67041 HCPLUS

DOCUMENT NUMBER: 106:67041

TITLE: Tetrahydrocarbazoles. Part II. Tricyclic inhibitors of gastric acid secretion

AUTHOR(S): Canas-Rodriguez, A.; Mateo Bernardo, A.

CORPORATE SOURCE: Chelsea Coll., Univ. London, London, SW3 6LX, UK

SOURCE: Anales de Quimica, Serie C: Quimica Organica y Bioquimica (1985), 81(3), 254-7

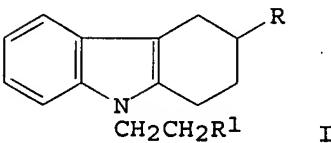
CODEN: AQSBD6; ISSN: 0211-1357

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 106:67041

GI

AB Tetrahydrocarbazoles I (R = Me, Et, CHMe₂, CMe₃, CH₂CMe₃; R₁ = NMe₂, NET₂, 1-pyrrolidinyl, 1-piperidyl) were prepared. Some of them showed gastric secretion inhibitory properties. Structure activity relationships of I were studied.

10558931.trn

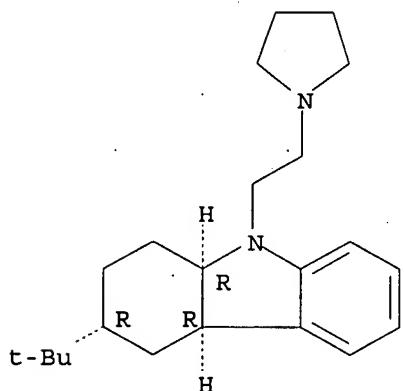
IT 106583-49-7P 106583-67-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and gastric secretion inhibition of)

RN 106583-49-7 HCPLUS

CN 1H-Carbazole, 3-(1,1-dimethylethyl)-2,3,4,4a,9,9a-hexahydro-9-[2-(1-pyrrolidinyl)ethyl]-, monohydrochloride, (3 α ,4 $\alpha\alpha$,9 $\alpha\alpha$)-(9CI) (CA INDEX NAME)

Relative stereochemistry.

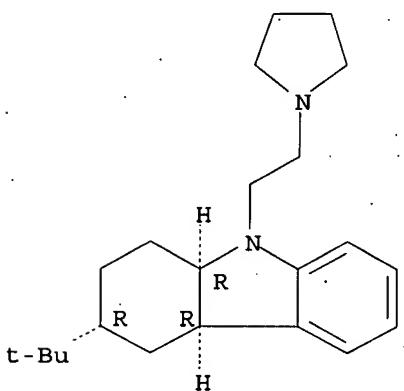


● HCl

RN 106583-67-9 HCPLUS

CN 1H-Carbazole, 3-(1,1-dimethylethyl)-2,3,4,4a,9,9a-hexahydro-9-[2-(1-pyrrolidinyl)ethyl]-, (3 α ,4 $\alpha\alpha$,9 $\alpha\alpha$)-(9CI) (CA INDEX NAME)

Relative stereochemistry.



L25 ANSWER 8 OF 15 HCPLUS COPYRIGHT 2007 ACS on STN

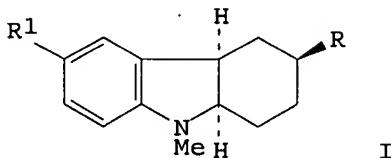
ACCESSION NUMBER: 1979:22056 HCPLUS

DOCUMENT NUMBER: 90:22056

TITLE: Substituent effects in saturated systems. An assessment of the transmission of substituent effects by the field, σ -inductive, and π -inductive

AUTHOR(S): effects in 3- and 6-substituted hexahydrocarbazoles
 Utley, James H. P.; Yeboah, Samuel O.
 CORPORATE SOURCE: Dep. Chem., Queen Mary Coll., London, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions
 2: Physical Organic Chemistry (1972-1999) (1978),
 (8), 766-70
 CODEN: JCPKBH; ISSN: 0300-9580

DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

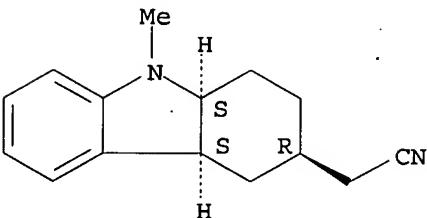


AB The basicities of the hexahydrocarbazoles I ($R = H, Me, CH_2OH, CH_2OMe, CH_2CN, R_1 = H; R = H, R_1 = Me, CMe_2CN, CH_2OH, CH_2OMe, CH_2CN$) were measured. For substituents of the type CH_2R_2 polar effects are analyzed in terms of the direct field effect operating from the 3-position (R) and the field and π -inductive effect operating in concert across the aromatic portion of the mol. (from R_1). Empirical correlations and the results of calcns. of ΔpK_a using the Kirkwood-Westheimer method show that the field effect is substantial but that relay by the π -inductive effect is greater by a factor of .apprx.2.5.

IT 68384-50-9
 RL: PRP (Properties)
 (basicity of, transmission of substituent effect in relation to)

RN 68384-50-9 HCPLUS
 CN 1H-Carbazole-3-acetonitrile, 2,3,4,4a,9,9a-hexahydro-9-methyl-,
 (3 α ,4 $\alpha\beta$,9 $\alpha\beta$)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

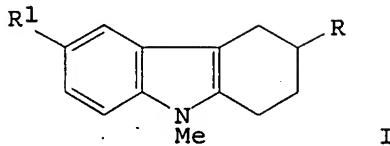


L25 ANSWER 9 OF 15 HCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1978:615158 HCPLUS
 DOCUMENT NUMBER: 89:215158
 TITLE: Preparation of a series of 3- and 6-substituted
 1,2,3,4-tetra- and 1,2,3,4,4a,9a-hexa-hydrocarbazoles
 AUTHOR(S): Utley, James H. P.; Yeboah, Samuel O.
 CORPORATE SOURCE: Dep. Chem., Queen Mary Coll., London, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions
 1: Organic and Bio-Organic Chemistry (1972-1999)
 (1978), (8), 888-92

DOCUMENT TYPE:
LANGUAGE:
GI

CODEN: JCPRB4; ISSN: 0300-922X

Journal
English



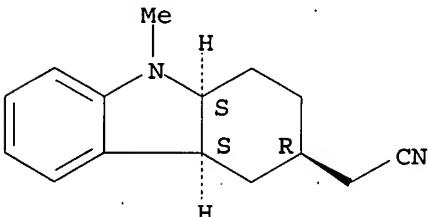
AB 4-Ethoxycarbonylcyclohexanone reacted with PhNMeNH₂ in AcOH-HCl under reflux to give 30% tetrahydrocarbazole I (R = CO₂H, R₁ = H), which on reductive methylation (NaH-MeI-DMF) gave 60% I (R = CH₂OMe, R₁ = H) and on p-tolylsulfonylation gave 75% I (R = CH₂O₃SC₆H₄Me-4, R₁ = H) (II). Treatment of II with NaCN-DMF gave 80% I (R = CH₂CN, R₁ = H) and II with pyridine.HCl-DMF gave 70% I (R = CH₂Cl). Bischler reaction of 2-chlorocyclohexanone (III) with 4-H₂NC₆H₄CO₂Et followed by methylation gave 80% I (R = H, R₁ = CO₂Et), which on LiAlH₄ reduction gave 70% I (R = H, R₁ = CH₂OH) (IV). Methylation of IV gave 50% I (R = H, R₁ = CH₂OMe). Bischler reaction of III with 4-H₂NC₆H₄CH₂CN gave 10% 6-cyanomethyl-1,2,3,4-tetrahydrocarbazole which on treatment with MeI gave 70% I (R = H, R₁ = CMe₂CN). Similarly, III with 4-MeNHC₆H₄CH₂CN gave 20% I (R = H, R₁ = CH₂CN). Hydrogenation of I (R = CH₂OH, CH₂OMe, CH₂CN, R₁ = H; R = H, R₁ = CO₂Et, CH₂OH, CH₂OMe, CH₂CN, CMe₂CN) gave the corresponding syn,cis and cis-hexahydrocarbazoles, resp.

IT 68384-50-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 68384-50-9 HCPLUS

CN 1H-Carbazole-3-acetonitrile, 2,3,4,4a,9,9a-hexahydro-9-methyl-,
(3 α ,4a β ,9a β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L25 ANSWER 10 OF 15 HCPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1971:448056 HCPLUS
DOCUMENT NUMBER: 75:48056
TITLE: Substituent effects in saturated systems. Basicity,
reactivity, and stereochemistry in 3- and
6-substituted cis-hexahydrocarbazoles
AUTHOR(S): Utley, J. H. P.; Smith, Alan
CORPORATE SOURCE: Queen Mary Coll., Univ. London, London, UK
SOURCE: Journal of the Chemical Society [Section] B: Physical
Organic (1971), (6), 1201-7
CODEN: JCSPAC; ISSN: 0045-6470

DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Rates of quaternization in MeCN and MeOH and pKa in H₂O and aqueous BuO(CH₂)₂OH were determined for N-methyl-cis-1,2,3,4,4a,9a-hexahydrocarbazoles substituted (Me₃C, Me, MeO) at the 3 and 6 positions. The decrease in basicity caused by 6-Me₃C, syn-3-Me and syn-3-Me₃C substitution is due to steric inhibition of general solvation of the conjugate acid, but this effect is offset by inhibition of H bonding to free base in the 3,3-di-Me derivative. The differences in rates of quaternization accompanying a change of solvent are due to steric effects on H bonding involving the N lone pair and MeOH.

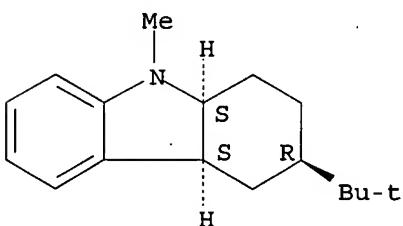
IT 25374-49-6

RL: RCT (Reactant); RACT (Reactant or reagent)
 (quaternization of, kinetics of)

RN 25374-49-6 HCAPLUS

CN Carbazole, 3β-tert-butyl-1,2,3,4,4aα,9aα-hexahydro-9-methyl- (8CI) (CA INDEX NAME)

Relative stereochemistry.



L25 ANSWER 11 OF 15 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1970:465901 HCAPLUS

DOCUMENT NUMBER: 73:65901

TITLE: Conformation of syn- and anti-3-substituted cis-hexahydrocarbazoles from nuclear magnetic resonance coupling constants.

AUTHOR(S): Shaw, Derek; Smith, Alan; Utley, J. H. P.

CORPORATE SOURCE: Dep. Chem., Queen Mary Coll., London, UK

SOURCE: Journal of the Chemical Society [Section] B: Physical Organic (1970), (6), 1161-5

CODEN: JCSPAC; ISSN: 0045-6470

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Double-irradiation expts. were used to interpret the NMR spectra of the methiodides of syn- and anti-3-substituted N-methyl-cis-hexahydrocarbazoles. The Karplus relation and conformational theory were used qual. to rationalize the characteristic splitting patterns and coupling consts. involving the ring junction protons, thus distinguishing between alternative conformations. For the syn series and the 3,3-dimethyl compound the alicyclic ring adopts a rigid shallow boat conformation. The anti compds. are probably conformationally mobile at probe temperature

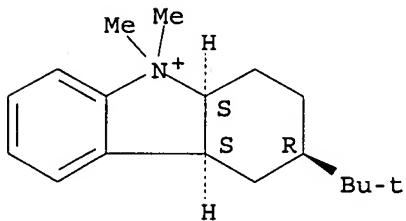
IT 25374-59-8

RL: PRP (Properties)
 (conformation of)

RN 25374-59-8 HCAPLUS

CN Carbazolium, 3β-tert-butyl-1,2,3,4,4aα,9aα-hexahydro-9,9-dimethyl-, iodide (8CI) (CA INDEX NAME)

Relative stereochemistry.



● I -

L25 ANSWER 12 OF 15 HCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1970:55144 HCPLUS

DOCUMENT NUMBER: 72:55144

TITLE: Configurational isomers of 3-substituted
cis-hexahydrocarbazoles

AUTHOR(S): Smith, Alan; Utley, J. H. P.

CORPORATE SOURCE: Dep. Chem., Queen Mary Coll., London, UK

SOURCE: Journal of the Chemical Society [Section] C: Organic
(1970), (1), 1-5

CODEN: JSOOAX; ISSN: 0022-4952

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The preparation and properties of cis-hexahydrocarbazoles (I) substituted (tert-Bu, Me, and MeO) at the 3- and 6-positions are described. The role of protonation in the smooth catalytic hydrogenation of tetrahydrocarbazoles in ethanol-aqueous fluoroboric acid was confirmed. Configurational isomers, defined as syn and anti, were identified in the 3-substituted series o I; their configurations were assigned according to conformational theory and NMR spectroscopic data.

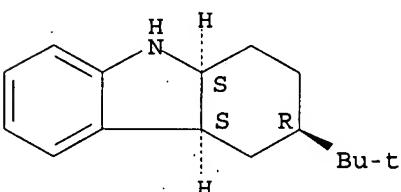
IT 25374-46-3P 25374-49-6P 25374-59-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 25374-46-3 HCPLUS

CN Carbazole, 3β-tert-butyl-1,2,3,4,4aa,9aa-hexahydro- (8CI)
(CA INDEX NAME)

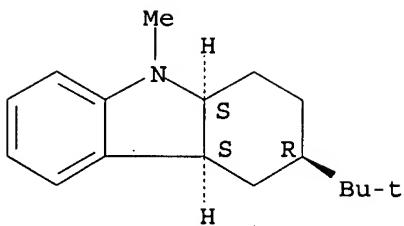
Relative stereochemistry.



RN 25374-49-6 HCPLUS

CN Carbazole, 3β-tert-butyl-1,2,3,4,4aa,9aa-hexahydro-9-
methyl- (8CI) (CA INDEX NAME)

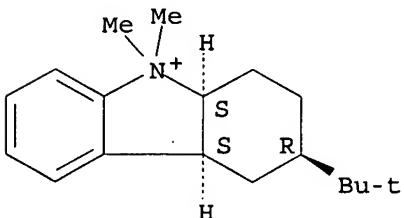
Relative stereochemistry.



RN 25374-59-8 HCPLUS

CN Carbazolium, 3 β -tert-butyl-1,2,3,4,4aa,9aa-hexahydro-9,9-dimethyl-, iodide (8CI) (CA INDEX NAME)

Relative stereochemistry.



● I-

L25 ANSWER 13 OF 15 HCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1966:35729 HCPLUS

DOCUMENT NUMBER: 64:35729

ORIGINAL REFERENCE NO.: 64:6602a-b

TITLE: Some studies of the formation and structure of melanins

AUTHOR(S): Swan, George Albert

CORPORATE SOURCE: Univ. Newcastle-upon-Tyne, UK

SOURCE: Rend. Accad. Sci. Fis. Mat. (Soc. Nazl. Sci., Napoli) (1964), 31, 212-31

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In addition to a literature review on the subject (25 references), studies are described of the formation of melanins (I), (a) enzymically, and (b) by autoxidn. from 2,3-(HO)2C6H3CH2CH(CO2H)NH2 (II) and 2,3-(HO)2C6H3CH2CH2NH2 (III). When II and III were labeled with D in the α or β position of the side chain and then converted to I, large retention of D was observed in the I. This suggests that the I are not polymers composed entirely of indole-5,6-quinone, but that they also contain uncyclized units of the precursors (or quinones derived from these) or (more probably) units of 2,3-dihydroindole-5,6-quinone. When I prepared from II-carboxy-14C was oxidized, the resulting pyrrole-2,3,5-tricarboxylic acid was radioactive while the pyrrole-2,3-dicarboxylic acid was inactive.

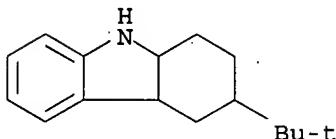
IT 6731-89-1

(Derived from data in the 7th Collective Formula Index (1962-1966))

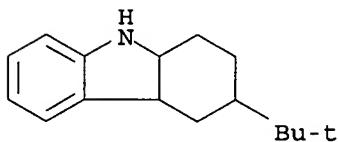
RN 6731-89-1 HCPLUS

CN 1H-Carbazole, 3-(1,1-dimethylethyl)-2,3,4,4a,9,9a-hexahydro- (9CI) (CA

INDEX NAME)



L25 ANSWER 14 OF 15 HCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1966:35728 HCPLUS
 DOCUMENT NUMBER: 64:35728
 ORIGINAL REFERENCE NO.: 64:6601g-h,6602a
 TITLE: Catalytic hydrogenation of indoles
 AUTHOR(S): Smith, A.; Utley, J. H. P.
 CORPORATE SOURCE: Queen Mary Coll., London
 SOURCE: Chemical Communications (London) (1965), (18), 427-8
 CODEN: CCOMA8; ISSN: 0009-241X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 64:35728
 GI For diagram(s), see printed CA Issue.
 AB Indoles (I), 1 g., were hydrogenated in EtOHHBF₄ solution over 0.01-0.5 g. PtO₂ at 1 atmospheric and room temperature to give quant. the corresponding indolines (R₁, R₂, and m.p. or b.p./mm. given): H, H, m. 95-6°; Me, H, m. 30-1°, H, Me, m. 54-6°; tert-Bu, H, m. 64-5°; H, tert-Bu, m. 75-7°.
 IT 6731-89-1P, Carbazole, 3-tert-butyl-1,2,3,4,4a,9a-hexahydro-
 RL: PREP (Preparation)
 (formation in 3-tert-butyl-1,2,3,4-tetrahydrocarbazole hydrogenation)
 RN 6731-89-1 HCPLUS
 CN 1H-Carbazole, 3-(1,1-dimethylethyl)-2,3,4,4a,9,9a-hexahydro- (9CI) (CA INDEX NAME)



L25 ANSWER 15 OF 15 HCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1952:57425 HCPLUS
 DOCUMENT NUMBER: 46:57425
 ORIGINAL REFERENCE NO.: 46:9616h-i,9617a-e
 TITLE: Imidazolines
 INVENTOR(S): Hartman, Max; Studer, Siegfried
 PATENT ASSIGNEE(S): C I B A Pharmaceutical Products, Inc.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|-------|-------|-----------------|-------|
| ----- | ----- | ----- | ----- | ----- |

US 2569415 19510925 US 1948-65067 19481213

AB 2-(9-Carbazolylalkyl)imidazolines (I) and their salts of inorg. or organic acids are prepared by treating a 9-carbazolealkanecarboxylic acid or its reactive acid derivative with a N-unsubstituted alkylenediamine or its reactive N-derivative I and their salts exhibit an action similar to that of adrenaline. 9-Carbazoleacetic acid 45 and $(CH_2NH_2)_2 \cdot H_2O$ 16 in warm alc. 300 parts by weight is mixed with 1 equivalent HCl in EtOH, the whole heated to about 230°, the EtOH distilled off, the mixture stirred 0.5 h., 28.4 parts P2O5 added, the temperature kept 1.5 h. at 230°, and the mass cooled, pulverized, and extracted with hot H₂O; the filtered solution yields 2-(9-carbazolylmethyl)-2-imidazoline, m. 232-234° (from EtOH). (HCl salt, m. 270-2°). Et 1,2,3,4,-tetrahydro-9-carbazoleacetate yields 2-(1,2,3,4-tetrahydro-9-carbazolylmethyl)-2-imidazoline, m. 180-1°; HCl salt, decompose 275-7.5°. 9-(Cyanomethyl)-1,2,8,4-tetrahydrocarbazole yields 2-(1,2,3,4-tetrahydro-9-carbazolylmethyl)-2-imidazoline, m. 132-3°, (HCl salt, m. 210-11° (decomposition). 9-(2-Cyanoethyl)carbazole produces 2-[2-(9-carbazolyl)ethyl]-2-imidazoline (HCl salt, m. 253°). 2-[2-(1,2,3,4-Tetrahydro-9-carbazolyl)ethyl]-2-imidazoline (HCl salt, m. 213-15°), is prepared from 9-(2-cyanoethyl)tetrahydrocarbazole. 2-Chlorocyclohexanone condensed with anilines substituted in the 4-position yields the 5,6,7,8-tetrahydrocarbazoles (II) substituted in the 3-position; the 3-PhO compound b0.1 209-10°, m. 141-3°. The II by reduction with Sn and concentrated HCl in EtOH yield the corresponding carbazolines: 3-Me, b0.5 114-15°; 3-MeO, b0.4 128-9°; 3-EtO, b0.18 132-4°; 3-PhO, b0.2 196-8°; 3-Cl, b0.38 134°, m. 62-4°. By treating the above carbazolines with trioxymethylene and aqueous KCN solution in glacial AcOH at 5-10° and then stirring 20 h. at room temperature may be prepared the following 9-(cyanomethyl)carbazolines: 3-Me, b0.32 157-8°; 3-MeO, m. 107-8°; 3-EtO, m. 102.5-3.5°; 3-PhO, m. 119.5-20.5°; 3-Cl, m. 81-2°. Upon dehydrogenation with chloranil in boiling xylene, the substituted 9-(cyanomethyl)carbazolines are converted into the corresponding 9-(cyanomethyl)carbazoles. 3-Methoxy-9-(cyanomethyl)carbazole (III), m. 116-17°, 17 refluxed 1 h. at a bath temperature of 220° with p-MeC₆H₄SO₃NH₃CH₂CH₂NH₂ 16.3 parts, the crystalline product dissolved in dilute EtOH, the solution made alkaline to phenolphthalein with 5 N NaOH, the precipitated crystalline powder dissolved in CH₂Cl₂, the solution dried over KOH and the CH₂Cl₂ evaporated gives 91.3% 2-(3-methoxy-9-carbazolylmethyl)-2-imidazoline (IV), m. 182-3° (after distillation in a high vacuum and recrystn. from EtOH); HCl salt, m. 227-8°. Similarly, the following analogs of III yield the corresponding analogs of IV. 3-Me analog of III, 9-(cyanomethyl)carbazole, m. 141-2°; of IV, m. 171-2.5° (HCl salt, m. 271-3°). 3-EtO analog of III, m. 95-7°; of IV, m. 164-5° (HCl salt, m. 242-2.5°). 3-PhO analog of III, m. 105-6°; of IV, m. 172.5-3.5° (HCl salt, m. 271-2°). 3-Cl analog of III; of IV, m. 213-15° (HCl salt, m. 263-5°).

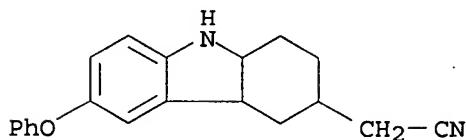
IT 854825-67-5P, 9-Carbazoleacetonitrile, 1,2,3,4,4a,9a-hexahydro-6-phenoxy- 854825-68-6P, 9-Carbazoleacetonitrile, 6-ethoxy-1,2,3,4,4a,9a-hexahydro- 854825-69-7P, 9-Carbazoleacetonitrile, 6-chloro-1,2,3,4,4a,9a-hexahydro- 855712-17-3P, 9-Carbazoleacetonitrile, 1,2,3,4,4a,9a-hexahydro-6-methoxy- 855712-19-5P, 9-Carbazoleacetonitrile, 1,2,3,4,4a,9a-hexahydro-6-methyl-

RL: PREP (Preparation)
(preparation of)

RN 854825-67-5 HCPLUS

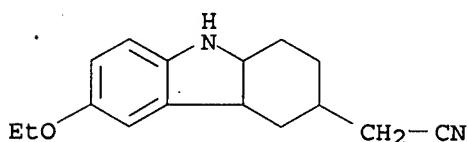
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CN 9-Carbazoleacetonitrile, 1,2,3,4,4a,9a-hexahydro-6-phenoxy- (5CI) (CA
INDEX NAME)



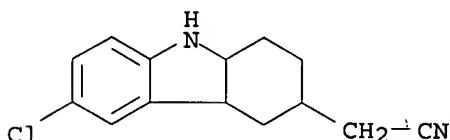
RN 854825-68-6 HCPLUS

CN 9-Carbazoleacetonitrile, 6-ethoxy-1,2,3,4,4a,9a-hexahydro- (5CI) (CA
INDEX NAME)



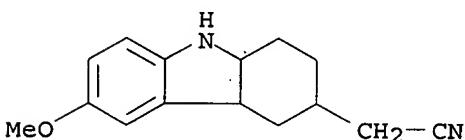
RN 854825-69-7 HCPLUS

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INDEX NAME)



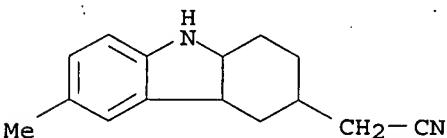
RN 855712-17-3 HCPLUS

CN 9-Carbazoleacetonitrile, 1,2,3,4,4a,9a-hexahydro-6-methoxy- (5CI) (CA
INDEX NAME)



RN 855712-19-5 HCPLUS

CN 9-Carbazoleacetonitrile, 1,2,3,4,4a,9a-hexahydro-6-methyl- (5CI) (CA
INDEX NAME)

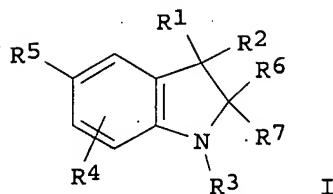


=> d l34 ibib abs hitstr tot

L34 ANSWER 1 OF 4 HCPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2000:790472 HCPLUS
 DOCUMENT NUMBER: 133:335158
 TITLE: Preparation of 3,3-substituted indolines as
 progesterone receptor antagonists
 INVENTOR(S): Ullrich, John W.; Fensome, Andrew; Zhi, Lin; Jones,
 Todd K.; Marschke, Keith B.; Tegley, Christopher M.
 PATENT ASSIGNEE(S): American Home Products Corporation, USA; Ligand
 Pharmaceuticals, Inc.
 SOURCE: PCT Int. Appl., 45 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|--------------|
| WO 2000066554 | A1 | 20001109 | WO 2000-US11464 | 20000501 <-- |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR,
CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,
ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,
LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE,
SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA,
ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 6417214 | B1 | 20020709 | US 2000-552352 | 20000419 <-- |
| CA 2371629 | A1 | 20001109 | CA 2000-2371629 | 20000501 <-- |
| EP 1175397 | A1 | 20020130 | EP 2000-930201 | 20000501 <-- |
| EP 1175397 | B1 | 20040818 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO | | | | |
| JP 2002543181 | T | 20021217 | JP 2000-615385 | 20000501 <-- |
| AT 273951 | T | 20040915 | AT 2000-930201 | 20000501 |
| PT 1175397 | T | 20050131 | PT 2000-930201 | 20000501 |
| ES 2226838 | T3 | 20050401 | ES 2000-930201 | 20000501 |
| US 2003008909 | A1 | 20030109 | US 2002-131379 | 20020424 <-- |
| US 6835744 | B2 | 20041228 | | |
| HK 1043986 | A1 | 20050401 | HK 2002-104852 | 20020628 |
| PRIORITY APPLN. INFO.: | | | US 1999-183061P | P 19990504 |
| | | | US 2000-552352 | A1 20000419 |
| | | | WO 2000-US11464 | W 20000501 |

OTHER SOURCE(S): MARPAT 133:335158
 GI

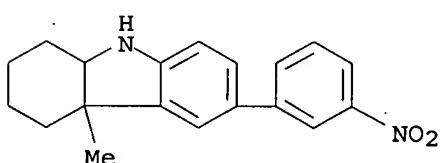


AB The title compds. [I; R1, R2 = H, OH, OAc, etc.; or R1 and R2 are joined to form a ring comprising CH₂(CH₂)nCH₂, CH₂CH₂CMe₂CH₂CH₂, O(CH₂)mCH₂, etc.; or R1 and R2 together comprise a double bond to CMe₂, C(cycloalkyl), O, C(cycloether); n = 0-5; m = 1-4; R3 = H, OH, NH₂, etc.; R4 = H, halo, CN, etc.; R5 = optionally substituted Ph, a 5-6 membered heterocycle, a 4- or 7-substituted indole, substituted benzothiophene; R6, R7 = H, Me, Et, etc.] which are progesterone receptor antagonists, and are useful in inducing contraception, and treating or preventing benign or malignant neoplastic disease, were prepared. Thus reacting 5-bromo-2,3,3-trimethyl-2,3-dihydro-1H-indole (preparation given) with 3-nitrophenylboronic acid in the presence of Pd(PPh₃)₄ afforded 82% I [R1, R2 = Me; R3, R4 = H; R5 = 3-O₂NC₆H₄; R6 = Me; R7 = H]. In general, compds. I were effective at 0.5-500 mg/kg/day.

IT 304468-33-5P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of 3,3-substituted indolines as progesterone receptor antagonists)

RN 304468-33-5 HCAPLUS

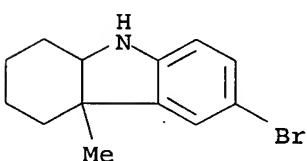
CN 1H-Carbazole, 2,3,4,4a,9,9a-hexahydro-4a-methyl-6-(3-nitrophenyl)- (9CI)
 (CA INDEX NAME)



IT 304468-40-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of 3,3-substituted indolines as progesterone receptor antagonists)

RN 304468-40-4 HCAPLUS

CN 1H-Carbazole, 6-bromo-2,3,4,4a,9,9a-hexahydro-4a-methyl- (9CI) (CA INDEX NAME)

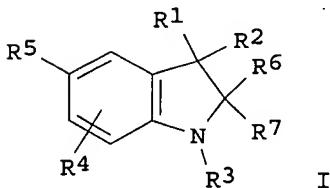


REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2000:790349 HCAPLUS
 DOCUMENT NUMBER: 133:350134
 TITLE: Preparation of 3,3-substituted indolines useful in contraceptive compositions
 INVENTOR(S): Grubb, Gary S.; Zhi, Lin; Jones, Todd K.; Tegley, Christopher M.; Ullrich, John W.; Fensome, Andrew; Wrobel, Jay E.; Edwards, James P.
 PATENT ASSIGNEE(S): American Home Products Corporation, USA; Ligand Pharmaceuticals, Inc.
 SOURCE: PCT Int. Appl., 53 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|--------------|
| WO 2000066166 | A1 | 20001109 | WO 2000-US11748 | 20000501 <-- |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR,
CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU,
ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU,
LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE,
SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA,
ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| US 6329416 | B1 | 20011211 | US 2000-552631 | 20000419 <-- |
| CA 2372591 | A1 | 20001109 | CA 2000-2372591 | 20000501 <-- |
| EP 1173211 | A1 | 20020123 | EP 2000-928667 | 20000501 <-- |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO | | | | |
| JP 2002543157 | T | 20021217 | JP 2000-615050 | 20000501 <-- |
| US 2002035099 | A1 | 20020321 | US 2001-977790 | 20011015 <-- |
| US 6503939 | B2 | 20030107 | | |
| PRIORITY APPLN. INFO.: | | | US 1999-183057P | P 19990504 |
| | | | US 2000-552631 | A1 20000419 |
| | | | WO 2000-US11748 | W 20000501 |

OTHER SOURCE(S): MARPAT 133:350134
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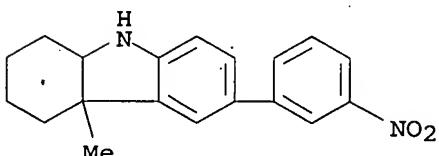


AB The title compds. [I; R₁, R₂ = H, OH, OAc, etc.; or R₁ and R₂ are joined to form a ring comprising CH₂(CH₂)nCH₂, CH₂CH₂CMe₂CH₂CH₂, O(CH₂)mCH₂, etc.; or R₁ and R₂ together comprise a double bond to CMe₂, C(cycloalkyl), O, C(cycloether); n = 0-5; m = 1-4; R₃ = H, OH, NH₂, etc.; R₄ = H, halo, CN, etc.; R₅ = optionally substituted Ph, a 5-6 membered heterocycle, a 4- or 7-substituted indole, substituted benzothiophene; R₆, R₇ = H, Me, Et, etc.] which are progesterone receptor antagonists, and are useful in inducing contraception, and treating or preventing benign or malignant neoplastic disease, were prepared. Thus reacting 5-bromo-2,3,3-trimethyl-2,3-dihydro-1H-indole (preparation given) with 3-nitrophenylboronic acid in the presence of Pd(PPh₃)₄ afforded 82% I [R₁, R₂ = Me; R₃, R₄ = H; R₅ = 3-O₂NC₆H₄; R₆ = Me; R₇ = H]. In general, compds. I were effective at 0.5-500 mg/kg/day..

IT 304468-33-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 3,3-substituted indolines as progesterone receptor antagonists)

RN 304468-33-5 HCPLUS

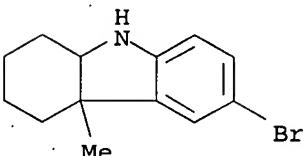
CN 1H-Carbazole, 2,3,4,4a,9,9a-hexahydro-4a-methyl-6-(3-nitrophenyl)- (9CI)
(CA INDEX NAME)

IT 304468-40-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 3,3-substituted indolines as progesterone receptor antagonists)

RN 304468-40-4 HCPLUS

CN 1H-Carbazole, 6-bromo-2,3,4,4a,9,9a-hexahydro-4a-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

6

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L34 ANSWER 3 OF 4 HCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:787188 HCPLUS

DOCUMENT NUMBER: 123:198832

TITLE: Tetracyclic condensed heterocyclic compounds for the treatment of senile dementia.

INVENTOR(S): Goto, Giichi; Ishihara, Yuji; Miyamoto, Masaomi

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: Eur. Pat. Appl., 53 pp.

CODEN: EPXXDW

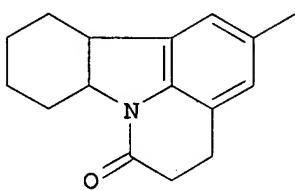
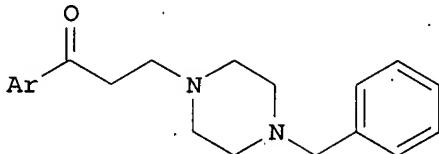
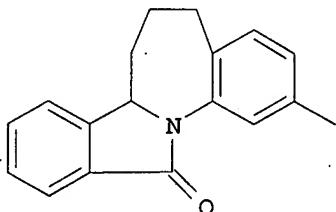
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|--------------|
| EP 655451 | A1 | 19950531 | EP 1994-118734 | 19941129 <-- |
| EP 655451 | B1 | 20010620 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE | | | | |
| US 5620973 | A | 19970415 | US 1994-330133 | 19941025 <-- |
| CA 2136913 | A1 | 19950531 | CA 1994-2136913 | 19941129 <-- |
| JP 07309835 | A | 19951128 | JP 1994-294754 | 19941129 <-- |
| AT 202354 | T | 20010715 | AT 1994-118734 | 19941129 <-- |
| US 5814642 | A | 19980929 | US 1996-681911 | 19960730 <-- |
| PRIORITY APPLN. INFO.: | | | JP 1993-299799 | A 19931130 |
| | | | JP 1994-55984 | A 19940325 |
| | | | US 1994-330133 | A3 19941025 |

OTHER SOURCE(S): CASREACT 123:198832; MARPAT 123:198832
GI $Q^1 =$  $Q^2 =$ 

I

AB Title compds. ArCO(CHR1)nY [Ar = (un)substituted tetracyclic fused heterocyclic group; R1 = H or (un)substituted hydrocarbyl; n = 1-10; Y = amino or N-containing saturated (un)substituted heterocyclic group] and their salts are claimed. The compds. show excellent cholinesterase inhibitory activity and monoamine uptake inhibitory activity, thus being useful as therapeutic and/or prophylactic medicaments for senile dementia and Alzheimer's disease, and also as antidepressants. For example, 1,2,3,4,4a,9a-hexahydrocarbazole underwent N-acylation by ClCH₂CH₂COCl, Friedel-Crafts cyclization by AlCl₃, and Friedel-Crafts acylation by treatment with both ClCH₂CH₂COCl and AlCl₃, to give pyridocarbazolone derivative ArCOCH₂CH₂Cl [Ar = Q1]. Reaction of the latter with 1-benzylpiperazine gave title compound I [Ar = Q1] as the di-HCl salt. The similarly prepared compound I [Ar = Q2] had IC₅₀ of 0.0164 μM for inhibition of rat cerebral cholinesterase in vitro, vs. 0.220 for physostigmine and 0.300 for THA. The same compound was also as potent as imipramine in a monoamine uptake inhibitor assay.

IT 167633-68-3P

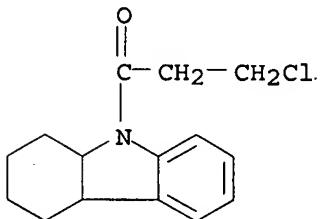
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(intermediate; preparation of tetracyclic heterocyclics for treatment of senile dementia)

RN 167633-68-3 HCPLUS

CN 1H-Carbazole, 9-(3-chloro-1-oxopropyl)-2,3,4,4a,9,9a-hexahydro- (9CI) (CA INDEX NAME)



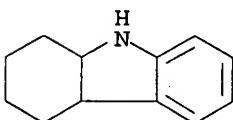
IT 1775-86-6, 1,2,3,4,4a,9a-Hexahydrocarbazole

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; preparation of tetracyclic heterocyclics for treatment of senile dementia)

RN 1775-86-6 HCPLUS

CN 1H-Carbazole, 2,3,4,4a,9,9a-hexahydro- (9CI) (CA INDEX NAME)



L34 ANSWER 4 OF 4 HCPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1981:47136 HCPLUS

DOCUMENT NUMBER: 94:47136

TITLE: Tetrahydrocarbazoles and pharmaceutical compositions for treating heart failure in mammals

INVENTOR(S): Mooradian, Aram

PATENT ASSIGNEE(S): Sterling Drug Inc., USA

SOURCE: U.S., 7 pp. Cont.-in-part of U.S. Ser. No. 465,238, abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

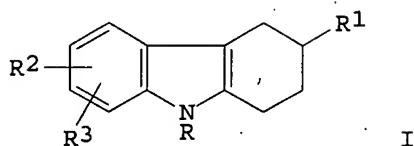
FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|--------------|
| US 4224335 | A | 19800923 | US 1976-651882 | 19760123 <-- |
| US 3642816 | A | 19720215 | US 1967-659606 | 19670810 <-- |
| US 3959309 | A | 19760525 | US 1973-425205 | 19731217 <-- |
| PRIORITY APPLN. INFO.: | | | US 1967-659606 | A2 19670810 |
| | | | US 1969-793545 | A2 19690123 |
| | | | US 1971-172206 | A2 19710816 |
| | | | US 1973-425205 | A2 19731217 |
| | | | US 1974-465238 | A2 19740429 |
| | | | CA 1968-10686 | A 19680124 |

OTHER SOURCE(S):
GI

MARPAT 94:47136



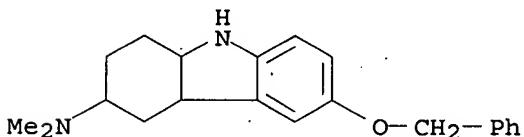
AB The carbazoles I (R = H, Me; R1 = NH2, EtNH, Me2N; R2 = 5-, 6-, 7-HO; R3 = H, 7-F, 7-HO) were prepared. Thus, m-PhCH2OC6H4NMeNH2.HCl was cyclized with 4-(dimethylamino)cyclohexanone to give I (R = Me, R1 = Me2N, R2 = 7-PhCH2O, R3 = H), which was debenzylated to give I (R = Me, R1 = Me2N, R2 = 7-HO, R3 = H). I underwent cardiotonic tests and were found useful for treatment of congestive heart failure in mammals.

IT 76243-30-6 76243-31-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(debenzylation of)

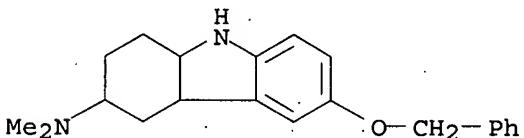
RN 76243-30-6 HCPLUS

CN 1H-Carbazol-3-amine, 2,3,4,4a,9,9a-hexahydro-N,N-dimethyl-6-(phenylmethoxy)- (9CI) (CA INDEX NAME)



RN 76243-31-7 HCPLUS

CN 1H-Carbazol-3-amine, 2,3,4,4a,9,9a-hexahydro-N,N-dimethyl-6-(phenylmethoxy)-, hydrochloride (9CI) (CA INDEX NAME)



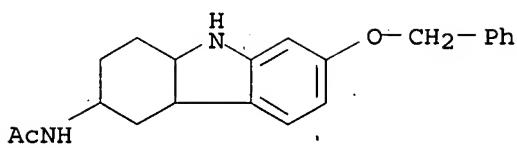
●x HCl

IT 76243-19-1P 76243-22-6P 76243-27-1P

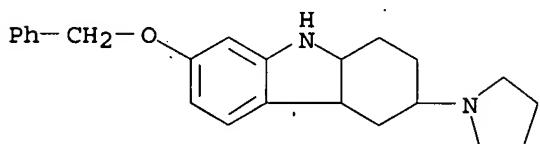
RL: RCT (Reactant); SPN (Synthetic preparation); PREP. (Preparation); RACT
(Reactant or reagent)
(preparation and debenzylation of)

RN 76243-19-1 HCPLUS

CN Acetamide, N-[2,3,4,4a,9,9a-hexahydro-7-(phenylmethoxy)-1H-carbazol-3-yl]- (9CI) (CA INDEX NAME)

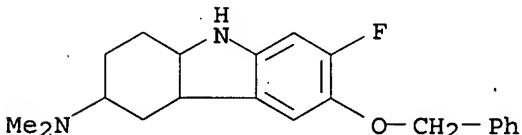


RN 76243-22-6 HCAPLUS
CN 1H-Carbazole, 2,3,4,4a,9,9a-hexahydro-7-(phenylmethoxy)-3-(1-pyrrolidinyl)-, hydrochloride (9CI) (CA INDEX NAME)



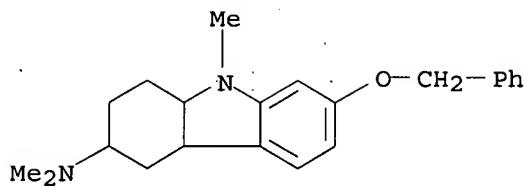
●x HCl

RN 76243-27-1 HCAPLUS
CN 1H-Carbazol-3-amine, 7-fluoro-2,3,4,4a,9,9a-hexahydro-N,N-dimethyl-6-(phenylmethoxy)-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

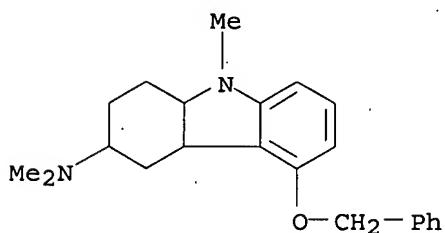
IT 76243-05-5P 76243-06-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolysis of)
RN 76243-05-5 HCAPLUS
CN 1H-Carbazol-3-amine, 2,3,4,4a,9,9a-hexahydro-N,N,9-trimethyl-7-(phenylmethoxy)-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

RN 76243-06-6 HCAPLUS

CN 1H-Carbazol-3-amine, 2,3,4,4a,9,9a-hexahydro-N,N,9-trimethyl-5-(phenylmethoxy)-, hydrochloride (9CI) (CA INDEX NAME)



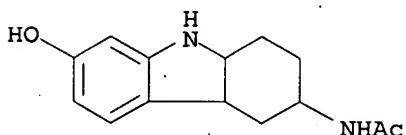
●x HCl

IT 76243-20-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

RN 76243-20-4 HCAPLUS

CN Acetamide, N-(2,3,4,4a,9,9a-hexahydro-7-hydroxy-1H-carbazol-3-yl)- (9CI) (CA INDEX NAME)



IT 76243-10-2P 76243-14-6P 76243-32-8P

76254-53-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

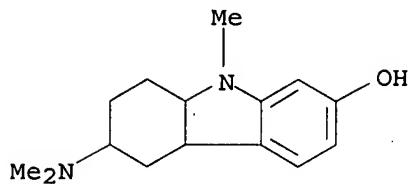
RN 76243-10-2 HCAPLUS

CN 1H-Carbazol-7-ol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro-9-methyl-, methanesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

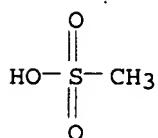
10558931.trn

CRN 76243-09-9
CMF C15 H22 N2 O



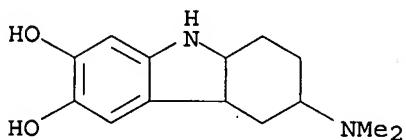
CM 2

CRN 75-75-2
CMF C H4 O3 S



RN 76243-14-6 HCAPLUS

CN 1H-Carbazole-6,7-diol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro-, hydrobromide (9CI) (CA INDEX NAME)



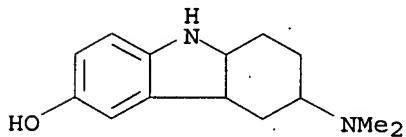
● x HBr

RN 76243-32-8 HCAPLUS

CN 1H-Carbazol-6-ol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro-, monomethanesulfonate (salt) (9CI) (CA INDEX NAME)

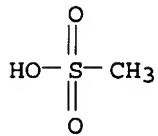
CM 1

CRN 76243-03-3
CMF C14 H20 N2 O

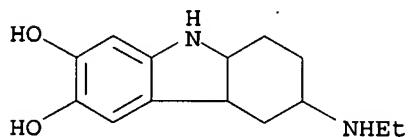


CM 2

CRN 75-75-2
CMF C H4 O3 S

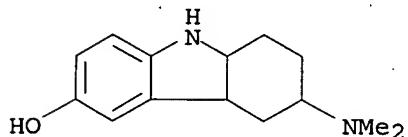


RN 76254-53-0 HCPLUS
CN 1H-Carbazole-6,7-diol, 3-(ethylamino)-2,3,4,4a,9,9a-hexahydro-, hydrobromide (9CI) (CA INDEX NAME)

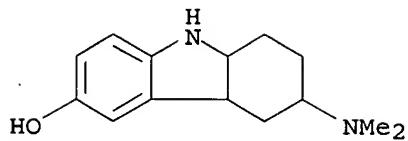


● x HBr

IT 76243-03-3P 76243-04-4P 76243-07-7P
76243-08-8P 76243-13-5P 76243-17-9P
76243-18-0P 76243-21-5P 76243-23-7P
76243-29-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, for treatment of congestive heart failure)
RN 76243-03-3 HCPLUS
CN 1H-Carbazol-6-ol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro- (9CI) (CA INDEX NAME)

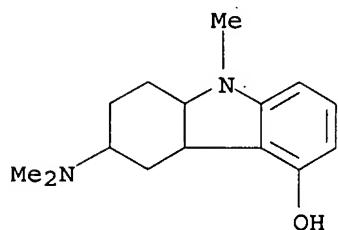


RN 76243-04-4 HCPLUS
CN 1H-Carbazol-6-ol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro-, hydrochloride (9CI) (CA INDEX NAME)



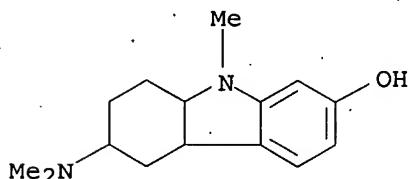
● x HCl

RN 76243-07-7 HCPLUS
CN 1H-Carbazol-5-ol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro-9-methyl-,
hydrochloride (9CI) (CA INDEX NAME)



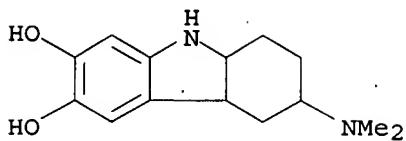
● x HCl

RN 76243-08-8 HCPLUS
CN 1H-Carbazol-7-ol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro-9-methyl-,
hydrochloride (9CI) (CA INDEX NAME)



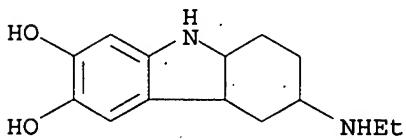
● x HCl

RN 76243-13-5 HCPLUS
CN 1H-Carbazole-6,7-diol, 3-(dimethylamino)-2,3,4,4a,9,9a-hexahydro-,
hydrochloride (9CI) (CA INDEX NAME)



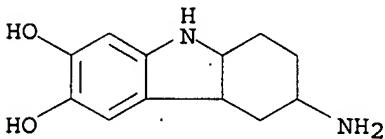
● x HCl

RN 76243-17-9 HCPLUS
CN 1H-Carbazole-6,7-diol, 3-(ethylamino)-2,3,4,4a,9,9a-hexahydro-, hydrochloride (9CI) (CA INDEX NAME)



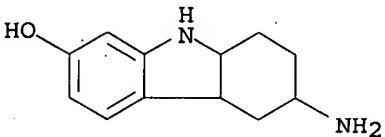
● x HCl

RN 76243-18-0 HCPLUS
CN 1H-Carbazole-6,7-diol, 3-amino-2,3,4,4a,9,9a-hexahydro-, hydrochloride (9CI) (CA INDEX NAME)



● x HCl

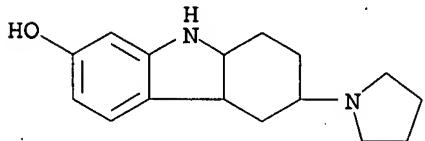
RN 76243-21-5 HCPLUS
CN 1H-Carbazol-7-ol, 3-amino-2,3,4,4a,9,9a-hexahydro-, hydrochloride (9CI) (CA INDEX NAME)



● x HCl

10558931.trn

RN 76243-23-7 HCAPLUS
CN 1H-Carbazol-7-ol, 2,3,4,4a,9,9a-hexahydro-3-(1-pyrrolidinyl)-, hydrochloride (9CI) (CA INDEX NAME)

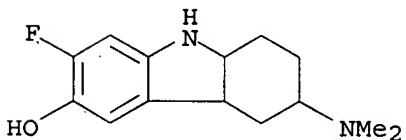


●x HCl

RN 76243-29-3 HCAPLUS
CN 1H-Carbazol-6-ol, 3-(dimethylamino)-7-fluoro-2,3,4,4a,9,9a-hexahydro-, monomethanesulfonate (salt) (9CI) (CA INDEX NAME)

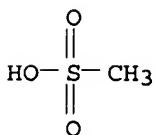
CM 1

CRN 76243-28-2
CMF C14 H19 F N2 O



CM 2

CRN 75-75-2
CMF C H4 O3 S



=> log y
COST IN U.S. DOLLARS

| | SINCE FILE
ENTRY | TOTAL
SESSION |
|---------------------|---------------------|------------------|
| FULL ESTIMATED COST | 120.93 | 1505.14 |

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

| | SINCE FILE
ENTRY | TOTAL
SESSION |
|---------------------|---------------------|------------------|
| CA SUBSCRIBER PRICE | -14.82 | -14.82 |

STN INTERNATIONAL LOGOFF AT 14:37:48 ON 10 AUG 2007